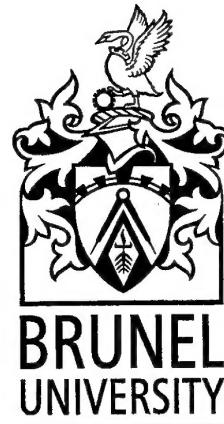


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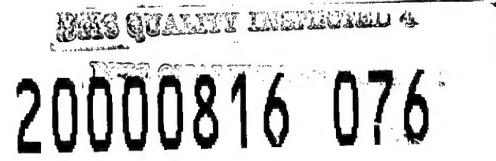
MAFELAP
1999

**Conference on the Mathematics
of Finite Elements and Applications**

22–25 June 1999

Summaries of Papers

**Brunel Institute of
Computational Mathematics**



MAFELAP 1999

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Contents of the MAFELAP 1999 Abstracts

List of all the abstracts	ii
List of the abstracts of the invited papers	xvii
List of the abstracts of the parallel session papers	xvii
List of the abstracts of the poster session papers	xix
List of the mini-symposium:	
Domain decomposition preconditioners	xix
A posteriori error estimation and reliability of FE computations	xx
Optimal and moving meshes	xx
Anisotropic mesh adaptivity for finite element methods	xxi
Boundary element methods for wave scattering problems	xxi
Computational modelling of forming processes	xxi
Adaptive methods for time dependent problems	xxii
Numerical treatment of singularities	xxii
Fluid structure interactions	xxii
Time Harmonic Maxwell problems	xxiii
Compressible flow	xxiii
Computational modelling of plasticity	xxiv
Finite and infinite elements for exterior problems	xxv
Adaptive and applications of domain decomposition methods	xxvi
Finite and boundary element methods for fluid structure interaction problems ..	xxvii
FEM and BEM in Biomechanics	xxvii
Adaptive methods for viscoelastic flow problems	xxviii
Mathematical modelling in geomechanics and tunnelling	xxviii
Hierarchical modelling	xxix
Finite element methods for eigenvalue problems	xxix
Multifield problems	xxx
Numerical analysis of contact mechanics and composite systems	xxx
Sparse approximation to integral and pseudo-differential operations; BEM/FEM applications	xxxi
Abstracts	1
Addresses of the authors	138
Author index	149

Simple A Posteriori Error Estimates for Transient Problems S. Adjerid, Ivo Babuška and J.E. Flaherty	
Mini-Symposium: Error estimation	1
Conditioning and Preconditioning of Boundary Element Equations on Non-Uniformly Refined Meshes Mark Ainsworth	
Mini-Symposium: Domain decomposition preconditioners	1
Nodally exact elements for axially loaded beam-on-elastic-foundation models J. E. Akin and D. R. Stephens	2
Fast Algorithms for Helmholtz Boundary Integral Equations Siamak Amini and Anthony Proffit	
Mini-Symposium: BEM for wave scattering	3
Contact Problems of Hyperelastic Membranes — Existence and numerical approximation of the solution H. Andrä, M. K. Warby and J. R. Whiteman	
Mini-Symposium: Modelling of forming processes	4
Robust solution of non-axisymmetric thermoforming: geometrical difficulties and their treatment H. Andrä, M. K. Warby and J. R. Whiteman	
Mini-Symposium: Modelling of forming processes	5
Anisotropic finite elements: local estimates and applications Thomas Apel	
Mini-Symposium: Anisotropic mesh adaptivity	5
Anisotropic mesh grading for the Stokes problem in domains with edges Thomas Apel and Serge Nicaise	
Mini-Symposium: Singularities	6
Some geometrical and interpolation estimates for hexahedral finite elements K. Arunakirinathar	6
Solving numerically the time-dependent Maxwell equations in domains with reentrant corners Franck Assous, Patrick Ciarlet Jr. and Jacques Segré	
Mini-Symposium: Maxwell problems	7
A fast transient infinite element scheme for unbounded wave problems R. J. Astley and J. A. Hamilton	
Mini-Symposium: Exterior problems	8
A posteriori error estimates, what we want and what we have Ivo Babuška	
Mini-Symposium: Error estimation	9

On the propagation of a plane crack in an isotropic 3D-body Michael Bach	
Mini-Symposium: Singularities	10
Optimal and Moving Meshes M. J. Baines	
Mini-Symposium: Moving meshes	11
Modeling of nonlinear hysteresis in elastomers H.T. Banks, G.A. Pinter, L.K. Potter, M.J. Gaitens and L.C. Yanyo	12
FEM for MHD K.E. Barrett	12
Improving Finite Element Methods for Fabricated Structures J. R. Barron	
Mini-Symposium: Contact mechanics	13
Finite Element Simulation in Orthopaedy Using MRI M. Bartoš, Z. Kestřánek jr, J. Nedoma, Z. Kestřánek and J. Stehlík	
Mini-Symposium: FEM and BEM in Biomechanics	14
Numerical solution of fluid-structure interaction using finite elements V. Beneš, Pavel Burda, P. Moses and Jaroslav Novotný	
Poster paper	15
Adaptivity and control of Finite Element Method for Plate Structures C. Benoit, P. Coorevits and J.-P. Pelle	16
Finite element approximation of a quadratic eigenvalue problem arising in damped fluid-structure interactions Alfredo Bermúdez, R. Durán, Rodolfo Rodríguez and J. Solomin	
Mini-Symposium: Eigenvalue problems	17
Finite element methods for fluid-structure vibration problems Alfredo Bermúdez and Rodolfo Rodríguez	
Mini-Symposium: Fluid structure interaction	18
An application of parallel high performance computing for analysis of stress fields induced by mining R. Blaheta, R. Kohut and J. Starý	
Mini-Symposium: Geomechanics and tunnelling	19
Finite element approximation for Maxwell's eigenproblem D. Boffi and L. Gastaldi	
Mini-Symposium: Eigenvalue problems	20
Nonstandard finite elements for Maxwell's eigenproblem in nonconvex domains D. Boffi and L. Gastaldi	
Mini-Symposium: Singularities	21

An accurate finite element solution of the biharmonic eigenproblem B.M. Brown, E.B. Davies, Peter K. Jimack and M.D. Mihajlović	22
An a posteriori error estimate for the Stokes problem in a polygonal domain Pavel Burda and Jaroslav Novotný	23
Large time-step operator splitting methods for nonlinear strongly degenerate convection-diffusion equations and applications to the theory of sedimentation-consolidation processes R. Bürger, S. Evje, K. Hvistendahl Karlsen and K.-A. Lie Mini-Symposium: Multifield problems	24
Valuation of financial options with probabilistic finite elements Gultekin Buyukyenerel	25
A Fast Two-Grid an Finite Section Method for an Acoustic Scattering Problem in the Half-Plane Simon N. Chandler-Wilde, M. Rahman and Christopher R. Ross Mini-Symposium: BEM for wave scattering	26
A model for grouted rockbolts, using a beam formulation T.-Y. Chao and M. B. Reed Mini-Symposium: Geomechanics and tunnelling	27
A posteriori error estimates for spectral element solutions to viscoelastic flow problems Cédric Chauvière and Robert G. Owens Mini-Symposium: Viscoelastic flow problems	28
Modelling of Underground Excavation in Two-Phase Media Annamaria Cividini and Giancarlo Gioda Mini-Symposium: Geomechanics and tunnelling	29
Parallel Computation of Flow in Heterogeneous Media Modelled by Mixed Finite Elements K. A. Cliffe, Ivan G. Graham, R. Scheichl and L. Stals Mini-Symposium: Adaptive and applications of domain decomposition	30
Postprocessing of high-order accurate Galerkin methods in locally translation invariant meshes Bernardo Cockburn Mini-Symposium: Time dependent problems	31
Boundary Conditions and Layer technique for the Simulation of Electromagnetic Waves above a Lossy Medium F. Collino Mini-Symposium: Exterior problems	31
Error estimator for finite element analyses of unilateral contact problem P. Coorevits, P. Hild and J.-P. Pelle	32

Crack and screen asymptotics	
M. Costabel and M. Dauge	
Mini-Symposium: Singularities	33
Infinite element methods for elasto-acoustics: implementation aspects and computational performances	
Jean-Pierre Coyette, Jean-Louis Migeot, and Tiago Lima	
Mini-Symposium: Fluid structure interaction	34
FEM Application for Predicting Characteristics of Linear Actuator	
M. D. Cundev, L. B. Petkovska, V. N. Stoilkov and G. V. Cvetkovski	34
Solution of Parabolic Equations by Backward Euler-Mixed Finite Element Methods on a Dynamically Changing Mesh	
Clint Dawson	
Mini-Symposium: Time dependent problems	36
Finite/Infinite Simulations for Maxwell's equations	
Leszek Demkowicz, W. Rachowicz and W. Cecot	
Mini-Symposium: Exterior problems	37
Finite element approximation of a coupling eigenvalue problem in 2D	
H. De Schepper and R. Van Keer	
Mini-Symposium: Eigenvalue problems	38
On High-Order Finite Element Modeling of Stiffened Shells for Structural Acoustics	
Saikat Dey	
Mini-Symposium: Fluid structure interaction	39
Use of 3D elements for an analysis of composite structures	
Jozef Dicky and Roman Minár	
Mini-Symposium: Contact mechanics	40
Duality Based Domain Decomposition with Adaptive Natural Coarse Grid for Contact Problems	
Z. Dostál, F. A. M. Gomez Neto and S. A. Santos	41
Variable Step Size Rosenbrock Schemes for the Adaptive Solution of Nonlinear Parabolic Systems	
B. Erdmann and J. Lang	42
Adaptive Finite Volume – Finite Element Schemes for Compressible Navier-Stokes Equations	
Miloslav Feistauer	
Mini-Symposium: Compressible flow	43
Effective solution of large symmetric eigenvalue problems by combined multi-grid and Rayleigh quotient methods	
Y. T. Feng, D. Peric and D. R. J. Owen	
Mini-Symposium: Eigenvalue problems	44

The method of Transport for convection-diffusion equations M. Fey, J. Maurer and R. Jeltsch Mini-Symposium: Compressible flow	45
Multiscale Models for Problems in Heterogeneous Media Jacob Fish Mini-Symposium: Heirarchical modelling	46
Far-field boundary conditions for finite element approximation of vascular flow problems Luca Formaggia, Fabio Nobile, Alfio Quarteroni and Alessandro Veneziani Mini-Symposium: Exterior problems	47
An enhanced error estimator on the constitutive relation for nonlinear time dependent problems L. Gallimard, P. Ladevèze and J.-P. Pelle Mini-Symposium: Error estimation	48
Boundary element methods for some nonlinear problems M. Ganesh and O. Steinbach Mini-Symposium: BEM for wave scattering	49
Combination of Mixed-FEM and DtN mappings for nonlinear exterior transmission problems Gabriel N. Gatica Mini-Symposium: Exterior problems	50
On applications of bounding energy theorems in computations of deformable systems Andrzej Gawecki Mini-Symposium: Modelling of plasticity	51
Fast Infinite Element Methods Klaus Gerdes Mini-Symposium: Exterior problems	52
Multilevel Evaluation of Boundary Integral Operators K. Giebermann Mini-Symposium: Fluid structure interaction	52
A survey on compression methods for boundary element matrices K. Giebermann and Michael Griebel Mini-Symposium: BEM for wave scattering	53
A hierarchy of optimal non-reflecting finite elements D. Givoli, A. Sidi and I. Patlashenko Mini-Symposium: Exterior problems	53
Numerical approximation of eigenvalue problems in integrated optics M. D. Gómez and P. Joly Mini-Symposium: Eigenvalue problems	54

Implementation of Fast Integration Methods in 3D Boundary Elements Ivan G. Graham	
Mini-Symposium: Sparse approximations	55
Body-Body Contact Solvers Based on Neumann DD Techniques B. Hackl and J. Schöberl	
Mini-Symposium: Adaptive and applications of domain decomposition	55
Trefftz infinite elements for acoustics I. Harari and P. E. Barbone	
Mini-Symposium: Exterior problems	56
Nodal Finite Elements for Maxwell's Equations: How to deal with geometric singularities Christophe Hazard and Stephanie Lohrengel	
Mini-Symposium: Maxwell problems	57
A Domain Splitting Method for Heat Conduction Problems In Composite Materials F.-K. Hebeker	
Mini-Symposium: Adaptive and applications of domain decomposition	58
The Fourier-finite-element method for treating edge singularities of some elliptic problems in axisymmetric domains B. Heinrich	
Mini-Symposium: Singularities	59
Contamination of soils and groundwater from volatile organic compounds Rainer Helmig	
Mini-Symposium: Multifield problems	60
Domain decomposition for high order boundary element methods Norbert Heuer	
Mini-Symposium: Domain decomposition preconditioners	60
Efficient implementation of hp finite element methods Stefan M. Holzer	
Mini-Symposium: Heirarchical modelling	61
A posteriori error analysis of stabilised finite element methods for hyperbolic problems Paul Houston	
Mini-Symposium: Moving meshes	62
Hybrid Coupled Finite-Boundary Element Methods for Elliptic Systems of Second Order G.C. Hsiao, E. Schnack and W.L. Wendland	
Mini-Symposium: Adaptive and applications of domain decomposition	63

A new mesh movement algorithm for finite element calculations II: Time dependent problems.

F. Hülsemann and Y. Tourigny	
Mini-Symposium: Moving meshes	63
Unified molecular dynamics and homogenization for bentonite behavior: Seepage and mass transportation	
Y. Ichikawa, K. Kawamura, M. Nakano, T. Seiki and N. Fujii	
Mini-Symposium: Geomechanics and tunnelling	64
New results on the stability of a coupled finite-infinite element approximation for exterior Helmholtz problems	
Frank Ihlenburg and Leszek Demkowicz	
Mini-Symposium: Exterior problems	65
A parallel domain decomposition iteration scheme for a heterogeneously modeled free boundary problem	
B. Jiang, J.C. Bruch, Jr. and J.M. Sloss	66
Finite Element Modelling of Helically Symmetric Structures	
W. G. Jiang and J. L. Henshall	
Mini-Symposium: Contact mechanics	67
On Optimal Node Location in the Finite Element Solution of Elliptic PDEs Using Unstructured Meshes in 2-D	
Peter K. Jimack	
Mini-Symposium: Moving meshes	68
A Viscoelastic Hybrid Shell Finite Element	
A. R. Johnson	69
Adaptive methods for finite-time blowup computations	
Ohannes Karakashain	
Mini-Symposium: Time dependent problems	69
On Robust Preconditioning in BEM with Graded Meshes	
Boris N. Khoromskij	
Mini-Symposium: Domain decomposition preconditioners	70
Approximation and Complexity Analysis for \mathcal{H} -Matrices in BEM/FEM Applications	
Wolfgang Hackbusch and Boris N. Khoromskij	
Mini-Symposium: Sparse approximations	70
Finite element methods for diffusion epidemic models with age-structured populations	
Mi-Young Kim	71
An Error Estimator for the Finite Element Analysis of Beams	
J.A. Kirby, M. K. Warby and J. R. Whiteman	71

Discontinuous Domain Decomposition Methods with Lagrange Multipliers for Elasticity Problems

Axel Klawonn

Mini-Symposium: Adaptive and applications of domain decomposition 72

Hierarchical Error Estimates

R. Kornhuber and R. Krause

Mini-Symposium: Domain decomposition preconditioners 72

Hierarchical Finite Element Methods in Fracture Mechanics

Roland Krause

Mini-Symposium: Heirarchical modelling 73

Tetrahedral partitions of acute type

Michal Křížek and Jana Pradlová 73

Convection dominated compressible flows

Dietmar Kroener

Mini-Symposium: Compressible flow 74

A multi-well problem for phase transformations

Mieczyslaw S. Kuczma

Mini-Symposium: Modelling of plasticity 75

Parallel Iterative Solvers for 3D Magnetic Field Problems

M. Kuhn 76

Adaptive Multi-level FEM Simulation for Coupled Field Problems

M. Kuhn, U. Langer, R. Lerch, W. Mühlhuber, S. Reitzinger, M. Schinnerl and J. Schöberl

Poster paper 76

A posteriori error estimation for anisotropic tetrahedral finite element meshes

G. Kunert

Mini-Symposium: Anisotropic mesh adaptivity 77

Boundary element analysis of the contact conditions between ceramic-coated mechanical components

L. A. de Lacerda and L. C. Wrobel

Mini-Symposium: Contact mechanics 78

Solving Short Wave Problems Using Special Finite Elements

O. Lagrouche and P. Bettess

Mini-Symposium: Exterior problems 78

Mathematical Scientific Computing Tools for 3D Magnetic Field Problems

U. Langer, M. Kuhn and J. Schöberl

INVITED PAPER 79

Finite Element Modelling of the Plug Assisted Thermoforming Process	
J. Lappin	
Mini-Symposium: Modelling of forming processes	80
Discrete Least Squares for Hyperbolic Equations and Systems Incorporating Mesh Movement	
S. J. Leary	
Mini-Symposium: Moving meshes	80
<i>hp</i> -adaptive Finite Element Methods for Viscoelastic Flow Calculations	
V. Legat	
Mini-Symposium: Viscoelastic flow problems	81
On the Fourier-boundary element method for elliptic problems with edge singularities	
J. M.-S. Lubuma, Serge Nicaise and L. Paquet	
Mini-Symposium: Singularities	82
Finite element method with optimal basic functions	
Oleg Lytvyn	83
A Unified Inverse Finite Element Strategy for Parameter Identification of Coupled Problems	
R. Mahnken	
Mini-Symposium: Modelling of plasticity	84
Mortar element method for boundary element discretizations of elliptic problems	
Matthias Maischak	
Mini-Symposium: Singularities	85
Efficient solution algorithms for simultaneous multiple frequency analysis of exterior acoustics problems	
M. Malhotra and P. M. Pinsky	
Mini-Symposium: Exterior problems	86
Boundary element methods and sound radiation – How to create explicit frequency dependent matrices	
Steffen Marburg	
Mini-Symposium: Fluid structure interaction	87
Coupling Procedures in Partitioned Methods for Fluid Structure Interaction	
Hermann G. Matthies and Jan Steindorf	
Mini-Symposium: Fluid structure interaction	88
Rapid Mesh Methods for Solving Inhomogeneous Biharmonic Integral Equations	
Anita Mayo	
Mini-Symposium: Sparse approximations	88
A fully discrete BEM–FEM method for the exterior Stokes problem in the plane	
S. Meddahi and F.-J. Sayas	
Mini-Symposium: Exterior problems	89

Integral Equation Methods for Scattering by Rough Surfaces A. Meier and T. Arens Mini-Symposium: BEM for wave scattering	90
<i>hp</i> -FEM for singularly perturbed reaction-diffusion equations in curvilinear polygons J. M. Melenk Mini-Symposium: Singularities	90
Computer Aided Design of Preforms for Injection Stretch Blow Moulding G.H. Menary, C.G. Armstrong, R.J. Crawford and J.P. McEvoy Mini-Symposium: Modelling of forming processes	91
A Poisson Pressure Approach to Finite Element Stress Analysis of Nearly Incompressible Materials S. Mijalkovic	91
4-Node Quad as Dirichlet type of Boundary Value Problem F. Molenkamp and C. B. Sharma	92
Analysis of Vibrations of Wetted Elastic Structures by FE-BE-Method P. Möller Mini-Symposium: Fluid structure interaction	93
Time domain unstructured grid approach for electromagnetic scattering in piecewise homogeneous media K. Morgan, O. Hassan, N. E. Pegg and N. P. Weatherill Mini-Symposium: Maxwell problems	94
Application of Finite Element method to periodic blood flow S. Natarajan and M. R. Mokhtarzadeh-Dehghan	95
Coupling boundary integrals — finite elements in Maxwell equations Jean-Claude Nédélec and Habib Ammari Mini-Symposium: Exterior problems	95
Flow Balancing in Extrusion Dies for Thin Walled Thermoplastic Profiles J. M. Nóbrega and O. S. Carneiro Mini-Symposium: Modelling of forming processes	96
Estimation of Modeling and Approximation Error in Multiscale Models of Heterogeneous Materials J. Tinsley Oden INVITED PAPER	97
Local Error Estimators and Adaptivity for Elastic Problems S. Ohnimus, M. Rüter, E. Stein and E. Walhorn Mini-Symposium: Heirarchical modelling	98

Some advanced computational strategies for the modelling of forming problems D. R. J. Owen, D. Peric, E. A. de Souza Neto and M. Dutko INVITED PAPER	99
Parallel domain decomposition procedure based on primal mixed finite element method Eun-Jae Park and Jungho Park	101
Multilevel methods for domain decomposition with locally refined meshes Joseph E. Pasciak Mini-Symposium: Adaptive and applications of domain decomposition	101
Simulation of Dental Implants Under Cyclic Loading Using a Voronoi Tessellation Based Frame Model of Trabecular Bone and p version finite elements for Compact Bone Abani K. Patra, Karl S. D'Souza, Michael Meenaghan and Dan de Tolla .	102
AFEAPI: Adaptive Finite Elements Application Programmers Interface Abani K. Patra, A. Laszloffy and J. Long	103
"Industrial Strength" Solvers – Domain Decomposition, Iterative and Multi-Level Sub-structuring Abani K. Patra Mini-Symposium: Domain decomposition preconditioners	104
Overlapping Schwarz Preconditioners for Unstructured Spectral and hp -Elements Luca F. Pavarino Mini-Symposium: Domain decomposition preconditioners	105
Domain Decomposition for Multiphase Flow: Interface Coupling of Different Numerical and Physical Models Malgorzata Peszynska Mini-Symposium: Adaptive and applications of domain decomposition	106
3D Magnetic Field Analysis in a Permanent Magnet Brushed Motor L. B. Petkovska, M. D. Cundev, G. V. Cvetkovski and V. N. Stoilkov	107
Semi-Lagrangian Finite Volume Methods for Viscoelastic Flow Problems Tim Phillips and A. J. Williams Mini-Symposium: Viscoelastic flow problems	108
Simulation of Three-Dimensional Flow of Blood in the Coronary Arteries Around Stenoses Based on the Finite Element Method Bernhard Quatember	109
Smooth approximation for the Verigin-Muskat problem and Saffman-Taylor instability Evgeniy Radkevich Mini-Symposium: Multifield problems	110

Hierarchical modelling using h- and p-version finite element approximations Ernst Rank and Alexander Düster Mini-Symposium: Heirarchical modelling	111
The dual-weighted residual method for error control and mesh adaptation in finite element methods Rolf Rannacher INVITED PAPER	111
A Posteriori Error Estimation and Mesh Adaptation for Finite Element Models in Elasto-Plasticity Rolf Rannacher and F. T. Suttmeier Mini-Symposium: Modelling of plasticity	112
Shape optimization for large deformation in elastoplasticity E. Rohan Mini-Symposium: Modelling of plasticity	112
Finite element modelling of smooth muscle tissues E. Rohan and R. Cimrman Mini-Symposium: FEM and BEM in Biomechanics	113
Nonconforming Methods for Maxwell Equations with application to Magnetotellurics Juan Santos and Fabio Zyserman Mini-Symposium: Maxwell problems	114
Variable order panel clustering Stefan Sauter Mini-Symposium: Sparse approximations	114
Wavelet approximation of Boundary Integral Operators Reinhold Schneider Mini-Symposium: Sparse approximations	115
Postprocessing of nonconforming FE solutions and a posteriori error estimation F. Schieweck Mini-Symposium: Error estimation	115
Superelements for Accurate Solutions to 2-D Elliptic Problems With Singularities on the Domain Boundary Bernard Schiff and Zohar Yosibash	116
Advanced Boundary Element Algorithms Ch. Schwab INVITED PAPER	117
Hierarchical Homogenization of Composites by the Generalized p-Version of the FEM Ch. Schwab Mini-Symposium: Heirarchical modelling	118

Simulations of Batch Sedimentation on the Particle Level Stefan Schwarzer, Kai Höfler, Bernd Wachmann and Hans Herrmann Mini-Symposium: Multifield problems	118
A posteriori error estimates in the adaptive finite element method of lines for parabolic equations K. Segeth Mini-Symposium: Error estimation	119
Modelling and finite element analysis of applied viscoelasticity problems Simon Shaw, A. R. Johnson and J. R. Whiteman INVITED PAPER	119
Domain decomposition iterative methods for time-harmonic Maxwell's equations based on nonconforming mixed finite elements Dongwoo Sheen, Taeyoung Ha and Ohin Kwon Mini-Symposium: Maxwell problems	120
Low energy basis preconditioning for unstructured spectral/hp element methods Spencer Sherwin and Mario Casarin Mini-Symposium: Domain decomposition preconditioners	120
An Efficient Implementation of the DtN Boundary Condition for Acoustic Scattering Joseph J. Shirron Mini-Symposium: Fluid structure interaction	121
On the coupling of finite and boundary elements O. Steinbach Mini-Symposium: FEM and BEM in Biomechanics	121
Computing fluid-structure interaction with two-dimensional Trefftz-type finite elements Malgorzata Stojek Mini-Symposium: Fluid structure interaction	122
The intrinsic norm finite element method for convection-diffusion problems Martin Stynes and R. Bruce Kellogg	123
<i>hp</i> -finite element methods for hyperbolic problems Endre Süli INVITED PAPER	123
Damage Mechanics and Plasticity Approaches for Tunnels in Jointed Rock G. Swoboda Mini-Symposium: Geomechanics and tunnelling	124
Streamline-diffusion method for nonconforming and conforming elements of lowest order L. Tobiska and G. Matthies	125

The ADER Approach for Constructing Advection Schemes of Arbitrary Accuracy E. F. Toro, R. C. Millington and L. A. M. Nejad Mini-Symposium: Compressible flow	126
A new moving mesh algorithm for finite element calculations I: variational problems Yves Tourigny Mini-Symposium: Moving meshes	126
Finite Element Matrices and <i>a priori</i> Error Estimates I.A. Tsukerman and A. Plaks Mini-Symposium: Anisotropic mesh adaptivity	127
A finite volume method for viscous compressible flows for low and high speed applications J. Vierendeels, K. Riemslagh, B. Merci and E. Dick Mini-Symposium: Compressible flow	128
An investigation of mesh quality and anisotropic mesh refinement for some finite element methods for fluid flow M. Walkley, Peter K. Jimack and M. Berzins Mini-Symposium: Anisotropic mesh adaptivity	129
A finite element based approach for nonlinear, unsteady fluid structure interaction problems Wolfgang A. Wall and Ekkehard Ramm Mini-Symposium: Fluid structure interaction	130
Contact Elements in the Stress Analysis of Intramedullary Nails C.J. Wang, A.L. Yettram, C.J. Brown, E.J. Huesler and P. Procter Mini-Symposium: Contact mechanics	131
Hybrid, neural-network/finite-element analysis of elastoplastic plates Zenon Waszczyzyn and Ewa Pabisek Mini-Symposium: Modelling of plasticity	132
Locally Conservative Algorithms for Flow Mary Fanett Wheeler INVITED PAPER	133
A Mortar Finite Element Method Using Dual Spaces for the Lagrange Multiplier Barbara Wohlmuth Mini-Symposium: Adaptive and applications of domain decomposition	133
On h -adaptive finite element methods contact problems P. Wriggers INVITED PAPER	134

Integral equation formulations for the low Reynolds number deformation of viscous fluids under surface tension	
L. C. Wrobel, A. R. M. Primo and H. Power	
INVITED PAPER	134
Lagrangian Finite Volume Analysis of Glass Pressing	
Kayhan Yigitler	135
Extracting Certain Quantities Associated with Three-Dimensional Singularities in Elliptic BVP by p-FEM	
Zohar Yosibash	
Mini-Symposium: Singularities	135
Boundary Layers in Thin Elastic 3-D Domains vis 2-D Hierarchic Plate Models	
Zohar Yosibash	
Mini-Symposium: Heirarchical modelling	136
Mathematical Analysis of Zienkiewicz-Zhu Patch Recovery Technique	
Zhimin Zhang	137

INVITED PAPERS

Mathematical Scientific Computing Tools for 3D Magnetic Field Problems U. Langer, M. Kuhn and J. Schöberl	79
Estimation of Modeling and Approximation Error in Multiscale Models of Heterogeneous Materials J. Tinsley Oden	97
Some advanced computational strategies for the modelling of forming problems D. R. J. Owen, D. Peric, E. A. de Souza Neto and M. Dutko	99
The dual-weighted residual method for error control and mesh adaptation in finite element methods Rolf Rannacher	111
Advanced Boundary Element Algorithms Ch. Schwab	117
Modelling and finite element analysis of applied viscoelasticity problems Simon Shaw, A. R. Johnson and J. R. Whiteman	119
<i>hp</i> -finite element methods for hyperbolic problems Endre Süli	123
Locally Conservative Algorithms for Flow Mary Fanett Wheeler	133
On <i>h</i> -adaptive finite element methods contact problems P. Wriggers	134
Integral equation formulations for the low Reynolds number deformation of viscous fluids under surface tension L. C. Wrobel, A. R. M. Primo and H. Power	134

PARALLEL SESSION PAPERS

Nodally exact elements for axially loaded beam-on-elastic-foundation models J. E. Akin and D. R. Stephens	2
Some geometrical and interpolation estimates for hexahedral finite elements K. Arunakirinathar	6
Modeling of nonlinear hysteresis in elastomers H.T. Banks, G.A. Pinter, L.K. Potter, M.J. Gaitens and L.C. Yanyo	12
FEM for MHD K.E. Barrett	12
Adaptivity and control of Finite Element Method for Plate Structures C. Benoit, P. Coorevits and J.-P. Pelle	16
An a posteriori error estimate for the Stokes problem in a polygonal domain Pavel Burda and Jaroslav Novotný	23
Valuation of financial options with probabilistic finite elements Gultekin Buyukyenerel	25

Error estimator for finite element analyses of unilateral contact problem P. Coorevits, P. Hild and J.-P. Pelle	32
FEM Application for Predicting Characteristics of Linear Actuator M. D. Cundev, L. B. Petkovska, V. N. Stoilkov and G. V. Cvetkovski	34
Duality Based Domain Decomposition with Adaptive Natural Coarse Grid for Contact Problems Z. Dostál, F. A. M. Gomez Neto and S. A. Santos	41
Variable Step Size Rosenbrock Schemes for the Adaptive Solution of Nonlinear Parabolic Systems B. Erdmann and J. Lang	42
A parallel domain decomposition iteration scheme for a heterogeneously modeled free boundary problem B. Jiang, J.C. Bruch, Jr. and J.M. Sloss	66
A Viscoelastic Hybrid Shell Finite Element A. R. Johnson	69
Finite element methods for diffusion epidemic models with age-structured populations Mi-Young Kim	71
An Error Estimator for the Finite Element Analysis of Beams J.A. Kirby, M. K. Warby and J. R. Whiteman	71
Tetrahedral partitions of acute type Michal Krížek and Jana Pradlová	73
Parallel Iterative Solvers for 3D Magnetic Field Problems M. Kuhn	76
Finite element method with optimal basic functions Oleg Lytvyn	83
A Poisson Pressure Approach to Finite Element Stress Analysis of Nearly Incompressible Materials S. Mijalkovic	91
4-Node Quad as Dirichlet type of Boundary Value Problem F. Molenkamp and C. B. Sharma	92
Application of Finite Element method to periodic blood flow S. Natarajan and M. R. Mokhtarzadeh-Dehghan	95
Parallel domain decomposition procedure based on primal mixed finite element method Eun-Jae Park and Jungho Park	101
Simulation of Dental Implants Under Cyclic Loading Using a Voronoi Tessellation Based Frame Model of Trabecular Bone and p version finite elements for Compact Bone Abani K. Patra, Karl S. D'Souza, Michael Meenaghan and Dan de Tolla ..	102
AFEAPI: Adaptive Finite Elements Application Programmers Interface Abani K. Patra, A. Laszloffy and J. Long	103

3D Magnetic Field Analysis in a Permanent Magnet Brushed Motor L. B. Petkovska, M. D. Cundev, G. V. Cvetkovski and V. N. Stoilkov	107
Simulation of Three-Dimensional Flow of Blood in the Coronary Arteries Around Stenoses Based on the Finite Element Method Bernhard Quatember	109
The intrinsic norm finite element method for convection-diffusion problems Martin Stynes and R. Bruce Kellogg	123
Streamline-diffusion method for nonconforming and conforming elements of lowest order L. Tobiska and G. Matthies	125
Lagrangian Finite Volume Analysis of Glass Pressing Kayhan Yigitler	135
Mathematical Analysis of Zienkiewicz-Zhu Patch Recovery Technique Zhimin Zhang	137

POSTER PAPERS

Numerical solution of fluid-structure interaction using finite elements V. Beneš, Pavel Burda, P. Moses and Jaroslav Novotný	15
Adaptive Multi-level FEM Simulation for Coupled Field Problems M. Kuhn, U. Langer, R. Lerch, W. Mühlhuber, S. Reitzinger, M. Schinnerl and J. Schöberl	76
Flow Balancing in Extrusion Dies for Thin Walled Thermoplastic Profiles J. M. Nóbrega and O. S. Carneiro	96

MINI-SYMPORIUM: Domain decomposition preconditioners

Organisers: Mark Ainsworth and Benji Guo

Conditioning and Preconditioning of Boundary Element Equations on Non-Uniformly Refined Meshes Mark Ainsworth	1
Domain decomposition for high order boundary element methods Norbert Heuer	60
On Robust Preconditioning in BEM with Graded Meshes Boris N. Khoromskij	70
“Industrial Strength” Solvers – Domain Decomposition, Iterative and Multi-Level Substructuring Abani K. Patra	104
Overlapping Schwarz Preconditioners for Unstructured Spectral and hp -Elements Luca F. Pavarino	105
Low energy basis preconditioning for unstructured spectral/ hp element methods Spencer Sherwin and Mario Casarin	120

MINI-SYMPOSIUM: A posteriori error estimation and reliability of FE computations

Organisers: Ivo Babuska, Lutz Tobiska, John Whiteman and Simon Shaw

Simple A Posteriori Error Estimates for Transient Problems

S. Adjerid, Ivo Babuška and J.E. Flaherty	1
A posteriori error estimates, what we want and what we have	
Ivo Babuška	9
An enhanced error estimator on the constitutive relation for nonlinear time dependent problems	
L. Gallimard, P. Ladevèze and J.-P. Pelle	48
Hierarchical Error Estimates	
R. Kornhuber and R. Krause	72
Postprocessing of nonconforming FE solutions and a posteriori error estimation	
F. Schieweck	115
A posteriori error estimates in the adaptive finite element method of lines for parabolic equations	
K. Segeth	119

MINI-SYMPOSIUM: Optimal and moving meshes

Organisers: Mike Baines

Optimal and Moving Meshes

M. J. Baines	11
A posteriori error analysis of stabilised finite element methods for hyperbolic problems	
Paul Houston	62
A new mesh movement algorithm for finite element calculations II: Time dependent problems.	
F. Hülsemann and Y. Tourigny	63
On Optimal Node Location in the Finite Element Solution of Elliptic PDEs Using Unstructured Meshes in 2-D	
Peter K. Jimack	68
Discrete Least Squares for Hyperbolic Equations and Systems Incorporating Mesh Movement	
S. J. Leary	80
A new moving mesh algorithm for finite element calculations I: variational problems	
Yves Tourigny	126

MINI-SYMPORIUM: Anisotropic mesh adaptivity for finite element methods

Organisers: Martin Berzins and Peter Jimack

Anisotropic finite elements: local estimates and applications Thomas Apel	5
A posteriori error estimation for anisotropic tetrahedral finite element meshes G. Kunert	77
Finite Element Matrices and <i>a priori</i> Error Estimates I.A. Tsukerman and A. Plaks	127
An investigation of mesh quality and anisotropic mesh refinement for some finite element methods for fluid flow M. Walkley, Peter K. Jimack and M. Berzins	129

MINI-SYMPORIUM: Boundary element methods for wave scattering problems

Organisers: Simon Chandler-Wilde

Fast Algorithms for Helmholtz Boundary Integral Equations Siamak Amini and Anthony Profit	3
A Fast Two-Grid an Finite Section Method for an Acoustic Scattering Problem in the Half-Plane Simon N. Chandler-Wilde, M. Rahman and Christopher R. Ross	26
Boundary element methods for some nonlinear problems M. Ganesh and O. Steinbach	49
A survey on compression methods for boundary element matrices K. Giebermann and Michael Griebel	53
Integral Equation Methods for Scattering by Rough Surfaces A. Meier and T. Arens	90

MINI-SYMPORIUM: Computational modelling of forming processes

Organisers: Jean-Loup Chenot, Jose Covas, Michael Warby and John Whiteman

Contact Problems of Hyperelastic Membranes — Existence and numerical approximation of the solution H. Andrä, M. K. Warby and J. R. Whiteman	4
Robust solution of non-axisymmetric thermoforming: geometrical difficulties and their treatment H. Andrä, M. K. Warby and J. R. Whiteman	5
Finite Element Modelling of the Plug Assisted Thermoforming Process J. Lappin	80
Computer Aided Design of Preforms for Injection Stretch Blow Moulding G.H. Menary, C.G. Armstrong, R.J. Crawford and J.P. McEvoy	91

MINI-SYMPORIUM: Adaptive methods for time dependent problems*Organisers: Bernard Cockburn and Clint Dawson*

Postprocessing of high-order accurate Galerkin methods in locally translation invariant meshes

Bernardo Cockburn	31
Solution of Parabolic Equations by Backward Euler-Mixed Finite Element Methods on a Dynamically Changing Mesh	
Clint Dawson	36
Adaptive methods for finite-time blowup computations	
Ohannes Karakashian	69

MINI-SYMPORIUM: Numerical treatment of singularities*Organisers: Martin Costabel and Monique Dauge*

Anisotropic mesh grading for the Stokes problem in domains with edges

Thomas Apel and Serge Nicaise	6
-------------------------------------	---

On the propagation of a plane crack in an isotropic 3D-body

Michael Bach	10
--------------------	----

Nonstandard finite elements for Maxwell's eigenproblem in nonconvex domains

D. Boffi and L. Gastaldi	21
--------------------------------	----

Crack and screen asymptotics

M. Costabel and M. Dauge	33
--------------------------------	----

The Fourier-finite-element method for treating edge singularities of some elliptic problems in axisymmetric domains

B. Heinrich	59
-------------------	----

On the Fourier-boundary element method for elliptic problems with edge singularities

J. M.-S. Lubuma, Serge Nicaise and L. Paquet	82
--	----

Mortar element method for boundary element discretizations of elliptic problems

Matthias Maischak	85
-------------------------	----

hp-FEM for singularly perturbed reaction-diffusion equations in curvilinear polygons

J. M. Melenk	90
--------------------	----

Superelements for Accurate Solutions to 2-D Elliptic Problems With Singularities on the Domain Boundary

Bernard Schiff and Zohar Yosibash	116
---	-----

Extracting Certain Quantities Associated with Three-Dimensional Singularities in Elliptic BVP by p-FEM

Zohar Yosibash	135
----------------------	-----

MINI-SYMPORIUM: Fluid structure interactions*Organisers: Mark Cross and Chris Bailey*

MINI-SYMPPOSEUM: Time Harmonic Maxwell problems

Organisers: Leszek Demkowicz and Peter Monk

Solving numerically the time-dependent Maxwell equations in domains with reentrant corners

Franck Assous, Patrick Ciarlet Jr. and Jacques Segré 7

Nodal Finite Elements for Maxwell's Equations: How to deal with geometric singularities

Christophe Hazard and Stephanie Lohrengel 57

Time domain unstructured grid approach for electromagnetic scattering in piecewise homogeneous media

K. Morgan, O. Hassan, N. E. Pegg and N. P. Weatherill 94

Nonconforming Methods for Maxwell Equations with application to Magnetotellurics

Juan Santos and Fabio Zyserman 114

Domain decomposition iterative methods for time-harmonic Maxwell's equations based on nonconforming mixed finite elements

Dongwoo Sheen, Taeyoung Ha and Ohin Kwon 120

MINI-SYMPPOSEUM: Compressible flow

Organisers: Miloslav Feistauer

Adaptive Finite Volume – Finite Element Schemes for Compressible Navier-Stokes Equations

Miloslav Feistauer 43

The method of Transport for convection-diffusion equations

M. Fey, J. Maurer and R. Jeltsch 45

Convection dominated compressible flows

Dietmar Kroener 74

The ADER Approach for Constructing Advection Schemes of Arbitrary Accuracy

E. F. Toro, R. C. Millington and L. A. M. Nejad 126

A finite volume method for viscous compressible flows for low and high speed applications

J. Vierendeels, K. Riemslagh, B. Merci and E. Dick 128

MINI-SYMPOSIUM: Computational modelling of plasticity*Organisers: Andrzej Gawecki and Mieczyslaw S.Kuczma*

On applications of bounding energy theorems in computations of deformable systems Andrzej Gawecki	51
A multi-well problem for phase transformations Mieczyslaw S. Kuczma	75
A Unified Inverse Finite Element Strategy for Parameter Identification of Coupled Problems R. Mahnken	84
A Posteriori Error Estimation and Mesh Adaptation for Finite Element Models in Elasto-Plasticity Rolf Rannacher and F. T. Suttmeier	112
Shape optimization for large deformation in elastoplasticity E. Rohan	112
Hybrid, neural-network/finite-element analysis of elastoplastic plates Zenon Waszczyszyn and Ewa Pabisek	132

MINI-SYMPOSIUM: Finite and infinite elements for exterior problems*Organisers: Dan Givoli*

A fast transient infinite element scheme for unbounded wave problems R. J. Astley and J. A. Hamilton	8
Boundary Conditions and Layer technique for the Simulation of Electromagnetic Waves above a Lossy Medium F. Collino	31
Finite/Infinite Simulations for Maxwell's equations Leszek Demkowicz, W. Rachowicz and W. Cecot	37
Far-field boundary conditions for finite element approximation of vascular flow prob- lems Luca Formaggia, Fabio Nobile, Alfio Quarteroni and Alessandro Veneziani .	47
Combination of Mixed-FEM and DtN mappings for nonlinear exterior transmission problems Gabriel N. Gatica	50
Fast Infinite Element Methods Klaus Gerdes	52
A hierarchy of optimal non-reflecting finite elements D. Givoli, A. Sidi and I. Patlashenko	53
Trefftz infinite elements for acoustics I. Harari and P. E. Barbone	56
New results on the stability of a coupled finite-infinite element approximation for ex- terior Helmholtz problems Frank Ihlenburg and Leszek Demkowicz	65
Solving Short Wave Problems Using Special Finite Elements O. Laghrouche and P. Bettess	78
Efficient solution algorithms for simultaneous multiple frequency analysis of exterior acoustics problems M. Malhotra and P. M. Pinsky	86
A fully discrete BEM-FEM method for the exterior Stokes problem in the plane S. Meddahi and F.-J. Sayas	89
Coupling boundary integrals — finite elements in Maxwell equations Jean-Claude Nédélec and Habib Ammari	95

MINI-SYMPORIUM: Adaptive and applications of domain decomposition methods

Organisers: Friedrich K. Hebeker, Ulrich Langer and Ronald Hoppe

Parallel Computation of Flow in Heterogeneous Media Modelled by Mixed Finite Elements

K. A. Cliffe, Ivan G. Graham, R. Scheichl and L. Stals 30

Body-Body Contact Solvers Based on Neumann DD Techniques

B. Hackl and J. Schöberl 55

A Domain Splitting Method for Heat Conduction Problems In Composite Materials

F.-K. Hebeker 58

Hybrid Coupled Finite-Boundary Element Methods for Elliptic Systems of Second Order

G.C. Hsiao, E. Schnack and W.L. Wendland 63

Discontinuous Domain Decomposition Methods with Lagrange Multipliers for Elasticity Problems

Axel Klawonn 72

Multilevel methods for domain decomposition with locally refined meshes

Joseph E. Pasciak 101

Domain Decomposition for Multiphase Flow: Interface Coupling of Different Numerical and Physical Models

Malgorzata Peszynska 106

A Mortar Finite Element Method Using Dual Spaces for the Lagrange Multiplier

Barbara Wohlmuth 133

MINI-SYMPORIUM: Finite and boundary element methods for fluid structure interaction problems*Organisers: Frank Ihlenburg*

Finite element methods for fluid-structure vibration problems

Alfredo Bermúdez and Rodolfo Rodríguez 18

Infinite element methods for elasto-acoustics: implementation aspects and computational performances

Jean-Pierre Coyette, Jean-Louis Migeot and Tiago Lima 34

On High-Order Finite Element Modeling of Stiffened Shells for Structural Acoustics

Saikat Dey 39

Multilevel Evaluation of Boundary Integral Operators

K. Giebermann 52

Boundary element methods and sound radiation – How to create explicit frequency dependent matrices

Steffen Marburg 87

Coupling Procedures in Partitioned Methods for Fluid Structure Interaction

Hermann G. Matthies and Jan Steindorf 88

Analysis of Vibrations of Wetted Elastic Structures by FE-BE-Method

P. Möller 93

An Efficient Implementation of the DtN Boundary Condition for Acoustic Scattering

Joseph J. Shirron 121

Computing fluid-structure interaction with two-dimensional Trefftz-type finite elements

Małgorzata Stojek 122

A finite element based approach for nonlinear, unsteady fluid structure interaction problems

Wolfgang A. Wall and Ekkehard Ramm 130

MINI-SYMPORIUM: FEM and BEM in Biomechanics*Organisers: Jiri Nedoma*

Finite Element Simulation in Orthopaedy Using MRI

M. Bartoš, Z. Kestřánek jr, J. Nedoma, Z. Kestřánek and J. Stehlík 14

Finite element modelling of smooth muscle tissues

E. Rohan and R. Cimrman 113

On the coupling of finite and boundary elements

O. Steinbach 121

MINI-SYMPOSIUM: Adaptive methods for viscoelastic flow problems*Organisers: Tim Phillips*

A posteriori error estimates for spectral element solutions to viscoelastic flow problems	
Cédric Chauvière and Robert G. Owens	28
<i>hp</i> -adaptive Finite Element Methods for Viscoelastic Flow Calculations	
V. Legat	81
Semi-Lagrangian Finite Volume Methods for Viscoelastic Flow Problems	
Tim Phillips and A. J. Williams	108

MINI-SYMPOSIUM: Mathematical modelling in geomechanics and tunnelling*Organisers: Martin Reed and Gunter Swoboda*

An application of parallel high performance computing for analysis of stress fields induced by mining	
R. Blaheta, R. Kohut and J. Starý	19
A model for grouted rockbolts, using a beam formulation	
T.-Y. Chao and M. B. Reed	27
Modelling of Underground Excavation in Two-Phase Media	
Annamaria Cividini and Giancarlo Gioda	29
Unified molecular dynamics and homogenization for bentonite behavior: Seepage and mass transportation	
Y. Ichikawa, K. Kawamura, M. Nakano, T. Seiki and N. Fujii	64
Damage Mechanics and Plasticity Approaches for Tunnels in Jointed Rock	
G. Swoboda	124

MINI-SYMPOSIUM: Hierarchical modelling*Organisers: Barna Szabo and Ernst Rank*

Multiscale Models for Problems in Heterogeneous Media

Jacob Fish	46
Efficient implementation of hp finite element methods	
Stefan M. Holzer	61
Hierarchical Finite Element Methods in Fracture Mechanics	
Roland Krause	73
Local Error Estimators and Adaptivity for Elastic Problems	
S. Ohnimus, M. Rüter, E. Stein and E. Walhorn	98
Hierarchical modelling using h- and p-version finite element approximations	
Ernst Rank and Alexander Düster	111
Hierarchical Homogenization of Composites by the Generalized p-Version of the FEM	
Ch. Schwab	118
Boundary Layers in Thin Elastic 3-D Domains via 2-D Hierarchic Plate Models	
Zohar Yosibash	136

MINI-SYMPOSIUM: Finite element methods for eigenvalue problems*Organisers: Roger Van Keer and Hennie de Schepper*

Finite element approximation of a quadratic eigenvalue problem arising in damped fluid-structure interactions	
Alfredo Bermúdez, R. Durán, Rodolfo Rodríguez and J. Solomin	17
Finite element approximation for Maxwell's eigenproblem	
D. Boffi and L. Gastaldi	20
An accurate finite element solution of the biharmonic eigenproblem	
B.M. Brown, E.B. Davies, Peter K. Jimack and M.D. Mihajlović	22
Finite element approximation of a coupling eigenvalue problem in 2D	
H. De Schepper and R. Van Keer	38
Effective solution of large symmetric eigenvalue problems by combined multi-grid and Rayleigh quotient methods	
Y. T. Feng, D. Peric and D. R. J. Owen	44
Numerical approximation of eigenvalue problems in integrated optics	
M. D. Gómez and P. Joly	54

MINI-SYMPOSIUM: Multifield problems*Organisers: Wolfgang Wendland*

Large time-step operator splitting methods for nonlinear strongly degenerate convection-diffusion equations and applications to the theory of sedimentation-consolidation processes

R. Bürger, S. Evje, K. Hvistendahl Karlsen and K.-A. Lie	24
Contamination of soils and groundwater from volatile organic compounds Rainer Helmig	60
Smooth approximation for the Verigin-Muskat problem and Saffman-Taylor instability Evgeniy Radkevich	110
Simulations of Batch Sedimentation on the Particle Level Stefan Schwarzer, Kai Höfler, Bernd Wachmann and Hans Herrmann	118

MINI-SYMPOSIUM: Numerical analysis of contact mechanics and composite systems*Organisers: Luis Wrobel and Leslie Henshall*

Improving Finite Element Methods for Fabricated Structures J. R. Barron	13
Use of 3D elements for an analysis of composite structures Jozef Dicky and Roman Minár	40
Finite Element Modelling of Helically Symmetric Structures W. G. Jiang and J. L. Henshall	67
Boundary element analysis of the contact conditions between ceramic-coated mechanical components L. A. de Lacerda and L. C. Wrobel	78
Contact Elements in the Stress Analysis of Intramedullary Nails C.J. Wang, A.L. Yettram, C.J. Brown, E.J. Huesler and P. Procter	131

MINI-SYMPORIUM: Sparse approximation to integral and pseudo-differential operations; BEM/FEM applications

Organisers: Ivan G. Graham, B. N. Khoromskij and S. A. Sauter

Implementation of Fast Integration Methods in 3D Boundary Elements

Ivan G. Graham	55
Approximation and Complexity Analysis for \mathcal{H} -Matrices in BEM/FEM Applications	
Wolfgang Hackbusch and Boris N. Khoromskij	70
Rapid Mesh Methods for Solving Inhomogeneous Biharmonic Integral Equations	
Anita Mayo	88
Variable order panel clustering	
Stefan Sauter	114
Wavelet approximation of Boundary Integral Operators	
Reinhold Schneider	115

MAFELAP 1999

Programme

Tuesday 22 June 1999

0900–1000: Registration in room H004.

H001

1000–1010 Welcome by the Vice Chancellor.

Chair: Luiz Wrobel

1010–1055

Locally Conservative Algorithms for Flow.

Mary Fanett Wheeler

1055–1115: COFFEE in H004

1115–1200

Modelling and finite element analysis of applied viscoelasticity problems.

Simon Shaw, A. R. Johnson and J. R. Whiteman

1200–1245

The dual-weighted residual method for error control and mesh adaptation in finite element methods.

Rolf Rannacher

1245–1400: LUNCH in the Newton room in the refectory

1400–1445, H001, Chair: P. Wriggers

Some advanced computational strategies for the modelling of forming problems.

D. R. J. Owen, D. Peric, E. A. de Souza Neto and M. Dutko

Tuesday 22 June 1999

H001 Time dependent problems Chair: Cockburn/Dawson	LC063 Multifield problems Chair: Wendland	LC065 Hierarchical modelling Chair: Rank	LC066 Modelling of forming processes Chair: Covas	LC067 Geomechanics and tunnelling Chair: Reed/Swoboda	H005 FEM and BEM in Biomechanics Chair: Nedoma
1450 Postprocessing of high-order accurate Galerkin methods in locally translation invariant meshes. Bernardo Cockburn	Simulations of Batch Sedimentation on the Particle Level. Stefan Schwarzter, Kai Höfler, Bernd Wachmann and Hans Herrmann	Hierarchical Homogenization of Composites by the Generalized p-Version of the FEM. Ch. Schwab	A Viscelastic Hybrid Shell Finite Element. A. R. Johnson	Damage Mechanics and Plasticity Approaches for Tunnels in Jointed Rock. G. Swoboda	On the coupling of finite and boundary elements. O. Steinbach
1520 Solution of Parabolic Equations by Backward Euler-Mixed Finite Element Methods on a Dynamically Changing Mesh. Clint Dawson	Multifield problems Large time-step operator splitting methods for nonlinear strongly degenerate convection-diffusion equations and applications to the theory of sedimentation-consolidation processes. R. Bürger, S. Evje, K. Hvistendahl Karlsen and K.-A. Lie	Multiscale Models for Problems in Heterogeneous Media. Jacob Fish	Modelling of nonlinear hysteresis in elastomers. H.T. Banks, G.A. Pinter, I.K. Potter, M.J. Gaffens and L.C. Yanyo	Parallel paper A model for grouted rockbolts, using a beam formulation. T.-Y. Chao and M. B. Reed	FEM and BEM in Biomechanics Finite element modelling of smooth muscle tissues. E. Rohan and R. Cimrman
Time dependent problems	Multifield problems	Heirarchical modelling	Heirarchical modelling	Geomechanics and tunnelling	FEM and BEM in Biomechanics Geomechanics and tunnelling

1550–1615: TEA in H004

Tuesday 22 June 1999

	H001 Anisotropic mesh adaptivity Chair: Jimack	LC0063 Multifield problems / Exterior problems Chair: Wendland/Giovilli	LC0065 Hierarchical modelling Chair: Rank	LC0066 Modelling of forming processes Chair: Kovas	LC0067 Geomechanics and tunnelling Chair: Reed/Swoboda	H005 FEM and BEM in Biomechanics Chair: Nedoma
1615	An investigation of mesh quality and anisotropic mesh refinement for some finite element methods for fluid flow. M. Walkley, Peter K. Jimack and M. Berzins	Contamination of soils and groundwater from volatile organic compounds. Rainer Helmig	Hierarchical Finite Element Methods in Fracture Mechanics. Roland Krause	Contact Problems of Hyperelastic Membranes — Existence and numerical approximation of the solution. H. Andr�, M. K. Warby and J. R. Whiteman	Unified molecular dynamics and homogenization for bentonite behaviour: Seepage and mass transportation. Y. Ichikawa, K. Kawamura, M. Nakano, T. Seiki and N. Fujii	Finite Element Simulation in Orthopaedics Using MRI. M. Barto�, Z. Kest��nek jr., J. Nedoma, Z. Kest��nek and J. Stehl�k
1645	Anisotropic finite elements: local estimates and applications. Thomas Apel	Multifield problems The intrinsic norm finite element method for convection-diffusion problems. Martin Stynes and R. Bruce Kellogg	Hierarchical modelling Local Error Estimators and Adaptivity for Elastic Problems. S. Ohnimus, M. R�iter, E. Stein and E. Wohorn	Modelling of forming processes Robust solution of non-axisymmetric thermoforming: geometrical difficulties and their treatment. H. Andr�, M. K. Warby and J. R. Whiteman	Geomechanics and tunnelling Modelling of Underground Excavation in Two-Phase Media. Annamaria Cividini and Giancarlo Gioda	FEM and BEM in Biomechanics Finite element methods for diffusion epidemic models with age-structured populations. Mi-Young Kim
1715	Anisotropic mesh adaptivity A. Posteriori error estimation for anisotropic tetrahedral finite element meshes. G. Kunert	Parallel paper Solving Short Wave Problems Using Special Finite Elements. O. Lagrouche and P. Bettess	Hierarchical modelling Boundary Layers in Thin Elastic 3-D Domains via 2-D Hierachic Plate Models. Zohar Yosibash	Modelling of forming processes Computer Aided Design of Pre-forms for Injection Stretch Blow Moulding. G.H. Menary, C.G. Armstrong, R.J. Crawford and J.P. McEvoy	Geomechanics and tunnelling Application of Finite Element method to periodic blood flow. S. Nararajan and M. R. Mokhtarzadeh-Delghan	Parallel paper
1745	Anisotropic mesh adaptivity Finite Element Matrices and a priori Error Estimates. I.A. Tsukerman and A. Plaks	Exterior problems Trefftz infinite elements for acoustics. I. Harari and P. E. Barbone	Hierarchical modelling Efficient implementation of hp finite element methods. Stefan M. Holzer	Modelling of forming processes Finite Element Modelling of the Plug Assisted Thermoforming Process. J. Lappin	Simulation of Dental Implants Under Cyclic Loading Using a Voronoi Tessellation Based Frame Model of Trabecular Bone and p -version finite elements for Compact Bone. Abani K. Patra, Karl S. D'Souza, Michael Meenaghan and Dan De Tolla	Parallel paper
1815	Anisotropic mesh adaptivity	Exterior problems	Hierarchical modelling	Modelling of forming processes Lagrangian Finite Volume Analysis of Glass Pressing. Kayhan Yigitler	Simulation of Three-Dimensional Flow of Blood in the Coronary Arteries Around Stenoses Based on the Finite Element Method. Bernhard Quatember	Parallel paper

1900: Buffet in the Newton room in the refectory.

Wednesday 23 June 1999

H001 Applications of domain decomps. Chair: Hebecker	LC063 Parallel session Chair: Wheeler	LC065 Sparse approximations Chair: Graham	LC066 Exterior problems Chair: Givoli	LC067 Parallel session Chair: Monk	H005 Parallel session Chair: Krizek
0900 A Domain Splitting Method for Heat Conduction Problems In Composite Materials. F.-K. Hebecker	Streamline-diffusion method for nonconforming and conforming elements of lowest order. L. Tobiska and G. Matthies	Variable order panel clustering. Stefan Sauter	Efficient solution algorithms for simultaneous multiple frequency analysis of exterior acoustics problems. M. Malhotra and P. M. Pinsky	FEM Application for Predicting Characteristics of Linear Actuator. J. D. Cundev, L. B. Petkovska, V. N. Stoykov and G. V. Cvetkovski	Nodally exact elements for axially loaded beam-on-elastic-foundation models. J. E. Akin and D. R. Stephens
0930 Multilevel methods for domain decomposition with locally refined meshes. Joseph E. Pasciak	Parallel Iterative Solvers for 3D Magnetic Field Problems. M. Kuhn	Wavelet approximation of Boundary Integral Operators. Reinhold Schneider	Boundary Conditions and Layer technique for the Simulation of Electromagnetic Waves above a Lossy Medium. F. Collino	3D Magnetic Field Analysis in a Permanent Magnet Brushed Motor. I. B. Petkovska, M. D. Cundev, G. V. Cvetkovski and V. N. Stoykov	4-Node Quad as Dirichlet type of Boundary Value Problem. F. Molentkamp and C. B. Sharma
1000 Hybrid Coupled Finite-Boundary Element Methods for Elliptic Systems of Second Order. G.C. Hsiao, E. Schnack and W.L. Wendland	Applications of domain decomps.	Variable Step Size Rosenbrock Schemes for the Adaptive Solution of Nonlinear Parabolic Systems. B. Erdmann and J. Lang	Sparse approximations Chair: Hackbusch and Boris N. Khoromskij	Exterior problems Chair: Gatica	Parallel paper A Poisson Pressure Approach to Finite Element Stress Analysis of Nearly Incompressible Materials. S. Mijalkovic
	Applications of domain decomps.	Parallel paper A Poisson Pressure Approach to Finite Element Stress Analysis of Nearly Incompressible Materials. S. Mijalkovic	Parallel paper A Poisson Pressure Approach to Finite Element Stress Analysis of Nearly Incompressible Materials. S. Mijalkovic	Parallel paper A Poisson Pressure Approach to Finite Element Stress Analysis of Nearly Incompressible Materials. S. Mijalkovic	Parallel paper A Poisson Pressure Approach to Finite Element Stress Analysis of Nearly Incompressible Materials. S. Mijalkovic

1030–1100: COFFEE in H004 and a Poster Session

Wednesday 23 June 1999
H001, Chair: Endre Süli

1100–1145

Estimation of Modeling and Approximation Error in Multiscale Models of Heterogeneous Materials.

J. Tinsley Oden

1145–1230

Advanced Boundary Element Algorithms.

Ch. Schwab

1230–1345: LUNCH in the Newton room in the refectory

1345–1445, H001, Chair: John Whiteman

Roland Glowinski

The Zienkiewicz Lecture. Roland Glowinski is also an IMA Distinguished Lecturer

H001 Applications of domain decompos. Chair: Hebecker	LC063 Eigenvalue problems Chair: Van Keer/De Schepper	LC065 Sparse approximations Chair: Graham	LC066 Exterior problems Chair: Girolli	LC067 Error estimation Chair: Babuška	H005 Parallel session Chair: Akiti
1450 Discontinuous Domain Decomposition Methods with Lagrange Multipliers for Elasticity Problems. Axel Klawonn	Finite element approximation of a coupling eigenvalue problem in 2D. H. De Schepper and R. Van Keer	Rapid Mesh Methods for Solving Inhomogeneous Biharmonic Integral Equations. Anita Mayo	Far-field boundary conditions for finite element approximation of vascular flow problems. Luca Formaggia, Fabio Nobile, Alfio Quarteroni and Alessandro Veneziani	Simple A Posteriori Error Estimates for Transient Problems. S. Adjerid, Ivo Babuška and J.E. Flaherty	Valuation of financial options with probabilistic finite elements. Gultekin Buyukyenerel
1520 Domain Decomposition for Multiphase Flow: Interface Coupling of Different Numerical and Physical Models. Małgorzata Peszynska	Applications of domain decompos. Chair: Hebeker	Eigenvalue problems Implementation of Fast Integration Methods in 3D Boundary Elements. Ivan G. Graham	Exterior problems A fast transient infinite element scheme for unbounded wave problems. R. J. Astley and J. A. Hamilton	Error estimation A posteriori error estimates, what we want and what we have. Ivo Babuška	Parallel paper Tetrahedral partitions of acute type. Michał Křížek and Jana Pradlová

Wednesday 23 June 1999

1550–1615: TEA in H004 and a Poster Session

	H001 Applications of domain decomps. Chair: Hebecker	LC063 Eigenvalue problems Chair: Van Keer/De Schepper	LC065 Singularities Chair: Costabel/Dauge	LC066 Exterior problems Chair: Givoli	LC067 Error estimation Chair: Babuška	H005 Fluid structure interactions Chair: Cross
1615	Body-Body Contact Solvers Based on Neumann DD Techniques. B. Hackl and J. Schöberl	Effective solution of large symmetric eigenvalue problems by combined multi-grid and Rayleigh quotient methods. Y. T. Feng, D. Peric and D. R. J. Owen	On the propagation of a plane crack in an isotropic 3D-body. Michael Bach	Finite/Infinite Simulations for Maxwell's equations. Leszek Demkowicz, W. Rachowicz and W. Cecot	A posteriori error estimates in the adaptive finite element method of lines for parabolic equations. K. Segeth	Flow through a model stented coronary artery. F.S. Henry
	<i>Applications of domain decomps.</i>		<i>Singularities</i>		<i>Error estimation</i>	
1645	A Mortar Finite Element Method Using Dual Spaces for the Lagrange Multiplier. Barbara Wohlmuth	An accurate finite element solution of the biharmonic eigenproblem. B.M. Brown, E.B. Davies, Peter K. Jimack and M.D. Mihajlović	Crack and screen asymptotics. M. Costabel and M. Dauge	Fast Infinite Element Methods. Klaus Gerdes	A Numerical Study of A Posteriori Error Estimators for Convection-Diffusion Equations. Volker John	Turbomachinery aeroelasticity: The present and the future. A. Seydel, M. Vahdati and M. Imregun
	<i>Applications of domain decomps.</i>		<i>Singularities</i>		<i>Error estimation</i>	
1715	Parallel Computation of Flow in Heterogeneous Media Modelled by Mixed Finite Elements. K. A. Cliffe, Ivan G. Graham, R. Scheichl and L. Stals	Finite element approximation of a quadratic eigenvalue problem arising in damped fluid-structure interactions. Alfredo Bermúdez, R. Durán, Rodolfo Rodríguez and J. Solomin	Extracting Certain Quantities Associated with Three-Dimensional Singularities in Elliptic BVP by p-FEM. Zohar Yosibash	A hierarchy of optimal non-reflecting finite elements. D. Givoli, A. Sidi and I. Patlashenko	Hierarchical Error Estimates. R. Kornhuber and R. Krause	Turbomachinery aeroelasticity: The present and the future. A. Seydel, M. Vahdati and M. Imregun
	<i>Applications of domain decomps.</i>		<i>Singularities</i>		<i>Error estimation</i>	
1745	Domain Decomposition Methods for the Euler Equations. T. Gonzalez and F. Nataf	Numerical approximation of eigenvalue problems in integrated optics. M. D. Gómez and P. Joly	Anisotropic mesh grading for the Stokes problem in domains with edges. Thomas Apel and Serge Nicaise	New results on the stability of a coupled finite-infinite element approximation for exterior Helmholtz problems. Frank Ihlenburg and Leszek Demkowicz	An enhanced error estimator on the constitutive relation for non-linear time dependent problems. L. Gallimard, P. Ladevèze and J.-P. Pelle	Fluid-Structure Interaction in Solidification Processes. C. Bailey, M. Cross, K. A. Pericleous, G. Taylor, S. Bounds, G. Moran and N. Croft
	<i>Applications of domain decomps.</i>		<i>Singularities</i>		<i>Error estimation</i>	
1815	Parallel domain decomposition procedure based on primal mixed finite element method. Eun-Jae Park and Jungho Park	The Fourier-finite-element method for treating edge singularities of some elliptic problems in axisymmetric domains. B. Heinrich			An integrated approach to a posteriori error estimation for conforming and nonconforming FE schemes. Lutz Angermann	Fluid-Structure Interaction in Solidification Processes. C. Bailey, M. Cross, K. A. Pericleous, G. Taylor, S. Bounds, G. Moran and N. Croft
	<i>Parallel paper</i>		<i>Singularities</i>		<i>Error estimation</i>	

1900: Dinner in the Newton room in the refectory.

Thursday 24 June 1999

	H001 Viscoelastic flow problems Chair: Phillips	LC063 Fluid structure interaction Chair: Ihlenburg	LC065 Singularities Chair: Costabel/Dauge	LC066 Parallel session	LC067 Domain decomp. preconditioners Chair: Ainsworth/Guo	H005 Parallel session
0900	A posteriori error estimates for spectral element solutions to viscoelastic flow problems. Cédric Chauvière and Robert G. Owens	Finite element methods for fluid-structure vibration problems. Alfredo Bermúdez and Rodolfo Rodríguez	Nonstandard finite elements for Maxwell's eigenproblem in non-convex domains. D. Boffi and L. Gastaldi	Finite element method with optimal basis functions. Oleg Lytvyn	"Industrial Strength" Solvers – Domain Decomposition, Iterative and Multi-Level Substructuring. Abani K. Patra	Adaptivity and control of Finite Element Method for Plate Structures. C. Benoit, P. Coorevits and J.-P. Pelle
	Viscoelastic flow problems hp-adaptive Finite Element Methods for Viscoelastic Flow Calculations. V. Legat	Fluid structure interaction Coupling Procedures in Partitioned Methods for Fluid Structure Interaction. Hermann G. Matthies and Jan Steindorf	Singularities Super-elements for Accurate Solutions to 2-D Elliptic Problems With Singularities on the Domain Boundary. Bernard Schiff and Zohar Yosibash	Parallel paper Some geometrical and interpolation estimates for hexahedral finite elements. K. Arunakirinathar	Overlapping Schwarz Preconditioners for Unstructured Spectral and hp-Elements. Luca F. Pavarino	Parallel paper An a posteriori error estimate for the Stokes problem in a polygonal domain. Pavel Burda and Jaroslav Novotný
0930	Viscoelastic flow problems Semi-Lagrangian Finite Volume Methods for Viscoelastic Flow Problems. Tim Phillips and A. J. Williams	Fluid structure interaction Analysis of Vibrations of Wetted Elastic Structures by FEBE-Method. P. Möller	Singularities On the Fourier-boundary element method for elliptic problems with edge singularities. J. M-S. Lubame, Serge Nicaise and L. Paquet	Parallel paper Low energy basis preconditioning for unstructured spectral/hp element methods. Spencer Sherwin and Mario Casarin	Parallel paper Error estimator for finite element analyses of unilateral contact problem. P. Coorevits, P. Hild and J.-P. Pelle	Parallel paper Domain decomp. preconditioners
1000	Viscoelastic flow problems Viscoelastic Finite Volume Methods for Viscoelastic Flow Problems.	Fluid structure interaction Viscoelastic flow problems	Singularities Singularities	Parallel paper Domain decomp. preconditioners		

1030–1100: COFFEE in H004 and a Poster Session

Thursday 24 June 1999

H001, Chair: Ivo Babuška

1100–1145

Mathematical Scientific Computing Tools for 3D Magnetic Field Problems.

U. Langer, M. Kuhn and J. Schöberl

1145–1230

On h -adaptive finite element methods in contact problems.

P. Wriggers

1230–1400: LUNCH in the Newton room in the refectory

1400–1445, H001, Chair: J. Tinsley Oden

hp -finite element methods for hyperbolic problems.

Endre Süli

	H001 Maxwell problems Chair: Demkowicz/Monk	LC063 Fluid structure interaction Chair: Ihlenburg	LC065 Singularities Chair: Costabel/Dauge	LC066	LC067 Domain decomp. preconditioners Chair: Ainsworth/Guo	H005
1450	Nodal Finite Elements for Maxwell's Equations: How to deal with geometric singularities. Christophe Hazard and Stephanie Lohrengel	Multilevel Evaluation of Boundary Integral Operators. K. Giebermann	<i>hp</i> -FEM for singularly perturbed reaction-diffusion equations in curvilinear polygons. J. M. Melenk		An Effective Preconditioner for the hp Version of the Finite Element Method in Two Dimensions. Benedict Guo	
1520	Maxwell problems	Fluid structure interaction	Singularities	Optimal Estimates for lower and upper bounds of the approximation errors in the p-FEM in the framework of the weighted Besov spaces. Benqi Guo	Domain decomp. preconditioners	Domain decomposition for high order boundary element methods. Norbert Heuer

1550–1615: TEA in H004 and a Poster Session

Thursday 24 June 1999

	H001 Maxwell problems Chair: Demkowicz/Monk	LC063 Fluid structure interaction Chair: Thelenburg	LC065 Singularities/Compressible flow Chair: Dauge/Felstrauer	LC066 Modelling of plasticity Chair: Gawecki/Kuczma	LC067 Domain decomp./preconditioners Chair: Ainsworth	H005 Parallel session Chair: Bruch
1615	Time domain unstructured grid approach for electromagnetic scattering in piecewise homogeneous media. K. Morgan, O. Hassan, N. E. Pegg and N. P. Weatherill	An Efficient Implementation of the DtN Boundary Condition for Acoustic Scattering. Joseph J. Shirron	Mortar element method for boundary element discretizations of elliptic problems. Matthias Maischak	Computational aspects of martensitic phase transition in elasto-plastic materials. E. Stein	On Robust Preconditioning in BEM with Graded Meshes. Boris N. Khoromskij	An Error Estimator for the Finite Element Analysis of Beams. J.A. Kirby, M. K. Warby and J. R. Whiteman
1645	Solving numerically the time-dependent Maxwell equations in domains with reentrant corners. Franck Assous, Patrick Ciarlet Jr. and Jacques Segré	Fluid structure interaction Infinite element methods for elasto-acoustics: implementation aspects and computational performances. Jean-Pierre Coyette, Jean-Louis Migeot and Tiago Lima	Singularities Adaptive Finite Volume – Finite Element Schemes for Compressible Navier-Stokes Equations. Milostav Felstrauer	Modelling of plasticity A multi-well problem for phase transformations. Mieczyslaw S. Kuczma	Domain decomp./preconditioners Conditioning and Preconditioning of Boundary Element Equations on Non-Uniformly Refined Meshes. Mark Ainsworth	Parallel paper AFEPPI: Adaptive Finite Elements Application Programmers Interface. Abani K. Patra, A. Laszloffy and J. Long
1715	Nonconforming Methods for Maxwell Equations with application to Magnetotellurics. Juan Santos and Fabio Zyserman	Fluid structure interaction Boundary element methods and sound radiation – How to create explicit frequency dependent matrices. Steffen Marburg	Compressible flow Convection dominated compressible flows. Dietmar Kroener	Modelling of plasticity A Unified Inverse Finite Element Strategy for Parameter Identification of Coupled Problems. R. Mahnken	Domain decomp./preconditioners Duality Based Domain Decomposition with Adaptive Natural Coarse Grid for Contact Problems. Z. Dostál, Neto F. A. M. Gomez and S. A. Santos	Parallel paper Mathematical Zienkiewicz-Zhu Patch Recovery Technique. Zhimin Zhang
1745	Domain decomposition methods for time-harmonic Maxwell equations. Alberto Valli	Fluid structure interaction Computing fluid-structure interaction with two-dimensional Trefftz-type finite elements. Małgorzata Stojek	Compressible flow The ADER Approach for Constructing Advection Schemes of Arbitrary Accuracy. E. F. Toro, R. C. Millington and L. A. M. Nejad	Modelling of plasticity Shape optimization for large deformation in elastoplasticity. E. Rohan	Parallel paper A parallel domain decomposition iteration scheme for a heterogeneously modeled free boundary problem. B. Jiang, J.C. Bruch, Jr. and J.M. Sloss	Reliability of a posteriori estimate techniques in finite element schemes. C. Carstensen and S. A. Funken
1815	Maxwell problems	Fluid structure interaction On High-Order Finite Element Modelling of Stiffened Shells for Structural Acoustics. Saikat Dey	Compressible flow The method of Transport for convection-diffusion equations. M. Fey, J. Maurer and R. Jeltsch	Modelling of plasticity Improving Finite Element Methods for Fabricated Structures. J. R. Barron	Contact mechanics Compressible flow	Parallel paper

1915: Pre-dinner sherry in the Bishops Bar in the refectory.

1930: Conference Dinner in the Newton room in the refectory.

Friday 25 June 1999

	H001 Moving meshes Chair: Baines	LC063 Contact mechanics Chair: Henshell/Wrobel	LC065 Compressible flow Chair: Feistauer	LC066 Modelling of plasticity Chair: Gawęcki/Kuczma	LC067 BEM for wave scattering Chair: Chandler-Wilde
0900	Optimal and Moving Meshes. M. J. Baines	Use of 3D elements for an analysis of composite structures. Jozef Dicky and Roman Minar	FEM for MHD. K.E. Barrett	Hybrid, neural-network/finite-element analysis of elastoplastic plates. Zenon Waszczyzyn and Ewa Pabisek	A survey on compression methods for boundary element matrices. K. Giebermann and Michael Griebel
0930	Moving meshes	Contact mechanics	Parallel paper	Modelling of plasticity	BEM for wave scattering
	Discrete Least Squares for Hyperbolic Equations and Systems Incorporating Mesh Movement. S. J. Leary	Boundary element analysis of the contact conditions between ceramic-coated mechanical components. L. A. De Lacerda and L. C. Wrobel	A finite volume method for viscous compressible flows for low and high speed applications. J. Vierendeels, K. Riemsdijk, B. Merci and E. Dick	A Posteriori Error Estimation and Mesh Adaptation for Finite Element Models in Elasto-Plasticity. Rolf Rannacher and F. T. Suttmeier	Boundary element methods for some nonlinear problems. M. Ganesh and O. Steinbach
1000	Moving meshes	Contact mechanics	Compressible flow	Modelling of plasticity	BEM for wave scattering
	On Optimal Node Location in the Finite Element Solution of Elliptic PDEs Using Unstructured Meshes in 2-D. Peter K. Jimack	Finite Element Modelling of Helically Symmetric Structures. W. G. Jiang and J. L. Henshall	On applications of bounding energy theorems in computations of deformable systems. Andrzej Gawecki	Modelling of plasticity	Integral Equation Methods for Scattering by Rough Surfaces. A. Meier and T. Arens
	Moving meshes	Contact mechanics			

1030–1100: COFFEE in H004

Friday 25 June 1999

H001, Chair: Frank Ihlenburg

1100–1145

Integral equation formulations for the low Reynolds number deformation of viscous fluids under surface tension.

L. C. Wrobel, A. R. M. Primo and H. Power

H001 Moving meshes Chair: Baines	LC063 Contact mechanics Chair: Henshell/Wrobel	LC065	LC066	LC067 BEM for wave scattering Chair: Chandler-Wilde
1150 A posteriori error analysis of stabilised finite element methods for hyperbolic problems. Paul Houston	Contact Elements in the Stress Analysis of Intranodular Nails. C.J. Wang, A.I. Yettram, C.J. Brown, E.J. Huesler and P. Procter			A Fast Two-Grid an Finite Section Method for an Acoustic Scattering Problem in the Half-Plane. Simon N. Chandler-Wilde, M. Rahman and Christopher R. Ross
1220 A new mesh movement algorithm for finite element calculations II: Time dependent problems. F. Hülsemann and Y. Tourigny	<i>Moving meshes</i> Contact mechanics			<i>BEM for wave scattering</i> Fast Algorithms for Helmholtz Boundary Integral Equations. Siamak Amini and Anthony Profit

1250–1400: LUNCH in the Newton room in the refectory

H001 Moving meshes Chair: Baines	LC063	LC065	LC066	LC067
1400 A new moving mesh algorithm for finite element calculations I: variational problems. Yves Tourigny				
1430				
1500				
1530				

1600–1620: TEA in H004
END OF THE CONFERENCE

SIMPLE A POSTERIORI ERROR ESTIMATES FOR TRANSIENT PROBLEMS

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We show that a posteriori estimates of spatial discretization errors of piecewise bi-polynomial finite element solutions of parabolic problems on meshes of square elements may be obtained from jumps in solution gradients at element vertices for odd-degree polynomial approximations and from local elliptic or parabolic problems for even-degree polynomials. These simple error estimates are asymptotically correct and extend in similar fashion to other finite element spaces. The key requirement is that the trial space contain all monomial terms of a given degree except for those in the principal coordinate directions. Computational results show that the error estimates are accurate, robust, and efficient for a wide range of problems, including some that are not supported by the present theory. These involve quadrilateral element meshes, problems with singularities, and nonlinear problems.

We describe related error estimation procedures for singularly perturbed convection-diffusion and hyperbolic problems. In one space dimension, these error estimates utilize superconvergence at the Radau points. The directional bias of the Radau points depends on the flow direction. Results are presented for several flow problems.

CONDITIONING AND PRECONDITIONING OF BOUNDARY ELEMENT EQUATIONS ON NON-UNIFORMLY REFINED MESHES

Mark Ainsworth

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The talk will discuss joint work with Bill McLean and Thanh Tran on the conditioning of the dense matrices that arise from the boundary element discretisation of boundary integral equations on surfaces in \mathbb{R}^3 when locally refined meshes are used as, for instance in an adaptive refinement algorithm. Bounds will be obtained for the dependence of the condition number on the order of the order m , the number of degrees of freedom N and the global mesh parameters h_{max} and h_{min} . The effect of using diagonal scaling to precondition the equations will be considered and shown to provide a simple but effective method for controlling the condition number. Numerical examples will be presented showing the bounds are sharp.

NODALLY EXACT ELEMENTS FOR AXIALLY LOADED BEAM-ON-ELASTIC-FOUNDATION MODELS

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In the oil and gas industry it is common to have very long drill-strings or off-shore pipelines that are subjected to axial loads and transverse bending while being supported on a linear or nonlinear foundation. The very long structure lengths make it desirable to have long elements. To obtain accurate results in that case it was decided to develop a family of nodally exact finite elements suitable for both static and dynamic applications. The ability to develop finite element solutions that are at least exact at the nodes was defined by Tong thirty years ago. Here it requires that the solution of a fourth-order ordinary differential equation be employed as the element interpolation functions. In this case they are transcendental functions. Their specific form depends on the local conditions of the element. The first deciding factor for the proper form is whether the axial loading is tension, zero, or compression. Solutions are developed for each case. Other options are whether the element is in contact with a supporting foundation. Axial and lateral foundations are allowed. Additional special cases are included for semi-infinite elements. The various interpolation forms are tabulated and illustrated graphically for varying proportions of axial load and foundation stiffness.

The element families have been verified against classic test problems. They are exact for linear foundation models. For nonlinear or piecewise linear foundations iterative techniques are shown to be effective with these elements. A common special case of a "compression only" foundation where a member may "lift off" and lose contact with the foundation is considered. The nodally exact forms differ in lift off regions, but iterations with constraints converge quickly for such problems.

References

- [1] Tong, P. "Exact Solution of Certain Problems by the Finite Element Method", AIAA Journal, v. 7, pp. 178-180, 1969.
- [2] Eisenberger, M. and Yankelevsky, D. Z., "Exact Stiffness Matrix for Beams on Elastic Foundations", Computers & Structures, v. 21, pp. 1355-1359, 1985.

FAST ALGORITHMS FOR HELMHOLTZ BOUNDARY INTEGRAL EQUATIONS

Siamak Amini and Anthony Profit

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Discretisation of boundary integral equations in general leads to fully populated complex valued and non-hermitian systems of linear equations. The cost of setting up the linear system, of dimension n say, is approximately $c_1 n^2$ with c_1 moderate to large. We then use iterative solvers from the Krylov subspace class which cost $c_3 n^2$ with c_3 small to moderate.

Several fast methods have been proposed which use an approximate coefficient matrix to reduce the computational cost [4, 1, 2]. We concentrate on those that use a separable approximation, leading to a low rank decomposition of submatrices of the coefficient matrix. In particular, we look at the multilevel fast multipole method for a hypersingular integral equation arising in the solution of the 2d Helmholtz equation [5, 3].

We give estimates for the error of the separable approximation for the diagonal form and for the error of the interpolation and anterpolation formulae used to communicate information between levels. From the requirement that this error is less than the discretisation error, we derive constraints for various parameters controlling the performance of the algorithm, leading to asymptotic complexity estimates.

References

- [1] G. Beylkin, R. Coifman, and V. Rokhlin. Fast wavelet transforms and numerical algorithms. *Comm. on Pure and Applied Math.*, 44:141–183, 1991.
- [2] W. Hackbusch and Z. P. Nowak. On the fast matrix multiplication in the boundary element method by panel clustering. *Numer. Math.*, 54:436–491, 1989.
- [3] C.C. Lu and W.C. Chew. A multilevel algorithm for solving a boundary integral equation of wave scattering. *Microwave and Optical Technology Letters*, 7(10):466–470, July 1994.
- [4] V. Rokhlin. Rapid solution of integral equations of classical potential theory. *J. Comp. Physics*, 60:187–207, 1985.
- [5] V. Rokhlin. Rapid solution of integral equations of scattering theory in two dimensions. *J. Comp. Physics*, 86:414–439, 1990.

CONTACT PROBLEMS OF HYPERELASTIC MEMBRANES

— EXISTENCE AND NUMERICAL APPROXIMATION OF THE SOLUTION

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We describe the pressure driven inflation of an incompressible isotropic hyperelastic membrane into a rigid mould by a variational inequality and consider the existence of a solution in the case of various strain energy functions of the Ogden form. By constructing relaxed strain energy functions, which are polyconvex and in some cases convex, we establish the existence of a solution of the constrained minimization problem for a limited range of pressures for the Mooney-Rivlin model and we establish the existence of a solution for all pressures for the Jones-Treloer model. We show that the more complicated Jones-Treloer strain-energy density is more appropriate than the usually used Mooney-Rivlin strain-energy density from the mathematical point of view. Also, the Jones-Treloer strain-energy density seems to have a better agreement with experimental results.

These theoretical results represent a necessary basis for the development of numerical approximations: Several strategies can be employed for the numerical solution of the variational inequality or constrained minimization problem, respectively. The most important methods proposed in literature are (a) penalty and Newton linearization, (b) convex minimization, (c) dual (augmented Lagrangian) and also (d) monotone multigrid methods. All of these methods can be applied for the relaxed strain-energy-density established in this work. The construction of a-priori error estimates is briefly explained. In a second paper at this conference, method (a) together with a continuation technique is explained in detail. The discretization of the considered problem is realized by using standard finite element approximations on adaptively refined meshes.

ROBUST SOLUTION OF NON-AXISYMMETRIC THERMOFORMING: GEOMETRICAL DIFFICULTIES AND THEIR TREATMENT

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A finite element model of the large constrained deformation of an incompressible isotropic hyperelastic membrane into a rigid mould will be described for modelling the deformation of thin polymeric sheets into moulds as occurs in thermoforming processes. This involves the usual finite deformation equations for membranes under quasi-static conditions when the forcing action is hydrostatic pressure, together with an algorithm to deal with the contact constraint as the sheet progressively sticks to the mould. Unfortunately in many instances thermoforming processes lead to situations where the sheet undergoes local compression, which causes it to fold. As a result of the above simulation procedures it is possible to investigate when such folding occurs and to propose ways of overcoming it. Some folding situations will be described, some possible remedies for overcoming these will be proposed and their effectiveness will be illustrated.

ANISOTROPIC FINITE ELEMENTS: LOCAL ESTIMATES AND APPLICATIONS

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We consider partial differential equations whose solution has (at least locally) different behaviour in different space directions. Applications include problems with edge and interface singularities in diffusion dominated problems (Poisson type equations) or with boundary layers arising in singularly perturbed problems.

The idea is to reflect this behaviour of the solution in a finite element approximation by using *anisotropic meshes* with a small mesh size in the direction of the rapid variation of the solution and a larger mesh size in the perpendicular direction.

In the talk an introduction into anisotropic finite elements is given. It covers anisotropic local interpolation error estimates and a-priori estimates of the discretization error for model problems.

The talk is based on the Habilitationsschrift of the author,
see Preprint SFB393/99-03, TU Chemnitz, January 1999,
<http://www.tu-chemnitz.de/~tap/papers/habil.html>.

ANISOTROPIC MESH GRADING FOR THE STOKES PROBLEM IN DOMAINS WITH EDGES

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The solution of the Stokes problem has in general anisotropic behaviour near edges with large interior angles. The solution varies much more rapidly perpendicularly to the edge (unbounded derivatives) than along the edge. Therefore it is an obvious idea to reflect this in the finite element discretization by using anisotropic meshes with a small mesh size in the direction of the rapid variation of the solution and a larger mesh size in the perpendicular direction.

In the talk we are concerned with a mixed discretization on a family of anisotropic meshes for a model problem. Several pairs of elements are discussed. Finally, the approximation properties are given for the case when Crouzeix-Raviart elements are used for the velocity and piecewise constants for the pressure.

SOME GEOMETRICAL AND INTERPOLATION ESTIMATES FOR HEXAHEDRAL FINITE ELEMENTS

K. Arunakirinathar

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The notion of the equivalent parallelipiped associated with a hexahedral is introduced. This parallelipiped is found to have some interesting geometric properties, and generates a natural means of defining a regular family of hexahedrals. It is shown furthermore that the *difference* between the equivalent parallelipiped and the hexahedral, measured in an appropriate way, is $O(h)$, where h is the length of the longer diagonal of the hexahedral. By making use of the properties of this parallelipiped together with the definition for regular family of hexahedrals we obtain some geometrical estimates and interpolation estimates.

SOLVING NUMERICALLY THE TIME-DEPENDENT MAXWELL EQUATIONS IN DOMAINS WITH REENTRANT CORNERS

Franck Assous^{1a}, Patrick Ciarlet Jr.^{2c}, and Jacques Segré^{1b}

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The aim of this presentation is to show that it is possible to solve Maxwell's equations in a non-convex domain with H^1 -conforming Finite Elements. We are concerned with the **time-dependent**¹ Maxwell equations in a bounded domain with either a Lipschitz polyhedral boundary (3D), or a polygonal boundary (2D). The choice of a Lagrange Finite Element can be justified by its precision, and by the simplicity of its implementation. When those equations are coupled with particle methods (leading to the Vlasov-Maxwell model), it is further justified by the need of having a numerical approximation which is continuous (in space), so as to increase the overall quality of the numerical solution.

As pointed out in the talk given by Stephanie Lohrengel and Christophe Hazard, when the domain Ω is not convex, the space V of solutions to the static or time-harmonic Maxwell equations with a perfectly conducting boundary can be split up into $V = V_R \overset{\perp}{\oplus} V_S$, where the subspace of \mathbf{H}^1 functions $V_R = V \cap \mathbf{H}^1(\Omega)$ is closed, and $V_S \neq \{0\}$. We call the method based on this (orthogonal) decomposition the **singular complement method**. Interestingly, the decomposition can be extended to the case of the time-dependent Maxwell equations, i. e. we can split up the electromagnetic field $\mathbf{v}(t)$: $\mathbf{v}(t) = \mathbf{v}_R(t) + \mathbf{v}_S(t)$. In addition, when the domain is 2D or 3D-axisymmetric, the dimension of V_S is finite. Thus one can actually write $\mathbf{v}(t) = \mathbf{v}_R(t) + \sum_{k=1}^{K} c_k(t) \mathbf{v}_S^k$, with $(\mathbf{v}_S^k)_{1 \leq k \leq K}$ a basis of V_S . Therefore, one simply has to add a numerically computed basis of V_S to the usual H^1 -conforming Finite Element which form a basis of V_R .

To emphasize those theoretical results, three numerical applications will be presented (in 2D). The first one is the study of a resonant cavity mode, the interest being that an analytic solution is available. The second one is the computation of the electromagnetic field induced by a current created by a particle beam; the numerical solution is compared to that obtained with a Finite Volume method. In the last example, an incoming wave inside a waveguide is computed (with Silver Müller absorbing boundary conditions), to illustrate the fact that this method works for different boundary conditions.

¹Note that, when computing the time-dependent solution, one has to solve an initial time-harmonic problem.

A FAST TRANSIENT INFINITE ELEMENT SCHEME FOR UNBOUNDED WAVE PROBLEMS

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Infinite elements provide a variable order non-reflecting boundary condition for unbounded solutions of Helmholtz equation. Since they are local in space, the resulting coefficient matrices retain sparsity when used in conjunction with conventional acoustic or structural finite elements in the near field. This is an important characteristic given that recent studies have indicated that sparsity is more significant than overall problem size in determining computational efficiency when the performance of infinite element and boundary element schemes are compared for large exterior problems [1, 2], particularly in the case of slender or flat radiators or scatterers, where the effectiveness of infinite element schemes can be further enhanced by the use of elements based on spheroidal or ellipsoidal coordinate systems [2, 3, 4]. Fully transient, infinite element schemes for unbounded problems have also been proposed [5, 6]. These are based on conjugated wave envelope elements. They are local in time and possess the same non-reflecting characteristics as their time-harmonic counterparts. When implemented with an implicit Newmark time integration scheme, such formulations offer highly efficient solutions for transient acoustics when compared to non-local BEM schemes [5]. In this paper, transient formulations of this type are modified by the use of an indirect solver to solve for the nodal pressures at each time step. This gives rapid convergence - typically after a few iterations provided that the time increment is of the same order as the wave transit time for a single element. Since it removes also the requirement for matrix reduction or factorisation and hence the need to store fill terms, all matrices can be stored in fully condensed format giving massive savings in computer storage requirements for large problems. The scheme proposed therefore has many of the characteristics of an explicit scheme - without requiring lumped masses or damping - while retaining the stability characteristics of the implicit formulation. Test solutions are presented for unbounded transient acoustical fields generated by the motion of a spherical surface started from rest. An unstructured acoustic FE mesh is used in the near field. Solutions for steady harmonic acoustical fields are also obtained by imposing harmonic excitation starting at $t = 0$ and stepping forward in time until a steady oscillatory solution is reached.

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A POSTERIORI ERROR ESTIMATES, WHAT WE WANT AND WHAT WE HAVE

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The talk will give reflections on a posteriori error estimations for finite element solutions of linear elliptic partial differential equations. It will discuss under what circumstances the estimators can be useble in the practice. Among others they should not include any generic constants,to be accurate for all accuracies i.e. not to be only asymptotic, lead to guaranteed upper and lower estimates etc and be well supported by the theory and computational tests of practical complexity.

ON THE PROPAGATION OF A PLANE CRACK IN AN ISOTROPIC 3D-BODY

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We consider the plane crack G in the elastic isotropic space \mathbb{R}^3 . Assuming that the symmetric normal loading P applied to the crack surfaces G^\pm opens the crack, the stress intensity factor (SIF) K_1 is a non-negative function on the crack front Γ while the mode 1 stress-strain state is realized at Γ . With the help of the Papkovich-Neuber representation, the 3-D elasticity problem in $\mathbb{R}^3 \setminus \overline{G}$ can be reduced to a scalar problem in the half-space.

We denote with s the arc-length on Γ and with $\kappa(s)$ the curvature of Γ (in the point s). If P is the critical loading (i.e. $\max K_1(s)$ is equal to the critical SIF K_{1c}), then an (positive) increment of the loading leads to the propagation of the crack. With

$$\Gamma(t) = \{y \in \partial\mathbb{R}_+^3 \cap U : r = h(t; s)\}$$

we denote the shape of the growing crack $G(t)$, where $h(t; s)$ describes the depth of the propagation along the normal to Γ at the point s and $t \geq 0$ is a fixed time-like parameter describing the increment of the loading $P(t; y) = P(y) + tP'(y)$. Both t and $h(t; s)$ are supposed to be small. Let us denote by $K_1(t; s)$ the SIF at $\Gamma(t)$ for the loading $P(t; y)$ on the crack surfaces $G^\pm(t)$, by K_{1c} the critical value of this SIF, by K'_1 the SIF corresponding to the increment of the loading P' and by $K_3(s)$ the ‘junior’ SIF.

Using the method of matched asymptotic expansions for the solution of the perturbed problem (at time t), the Irwin criterion leads to the variational inequality:

Find $H \in W_{2,+}^{\frac{1}{2}}(\Gamma)$ such that

$$\langle \beta_I H, X - H \rangle - \langle BH, X - H \rangle \geq \langle F_I, X - H \rangle \quad \forall X \in W_{2,+}^{\frac{1}{2}}(\Gamma),$$

where $\beta_I(s) = -\frac{1}{2} \frac{K_3(s)}{K_1(s)}$, $F_I(s) = K_1(s) - K_{1c} + t K'_1(s)$, $H(t; s) = K_1(s)h(t; s)$. B is a pseudo-differential operator of order 1.

The Griffith criterion says that the crack grows in such a way that the total energy $\Pi = U + S$ will be minimized, where U denotes the potential energy and S the surface energy of the system. Reformulating the minimization problem as variational inequality we get a similiar inequality as in the Irwin case:

Find $H \in W_{2,+}^{\frac{1}{2}}(\Gamma)$ such that

$$\langle \beta_G H, X - H \rangle - \langle BH, X - H \rangle \geq \langle F_G, X - H \rangle \quad \forall X \in W_{2,+}^{\frac{1}{2}}(\Gamma),$$

where $\beta_G(s) = -\frac{1}{2} \frac{K_3(s)}{K_1(s)} - \frac{\kappa(s)}{2} \left(1 - \frac{K_{1c}^2}{K_1^2(s)}\right)$, $F_G(s) = (K_1(s) - K_{1c}) \frac{K_1(s) + K_{1c}}{2K_1(s)} + t K'_1(s)$.

In the case of $\beta < 0$ ($\beta = \beta_I$ or β_G), $F \in L_2(\Gamma)$ ($F = F_I$ or F_G), the variational inequalities have a unique solution $H \in W_{2,+}^{\frac{1}{2}}(\Gamma)$, describing the propagation of the crack. The variational inequalities can be rewritten in form of equalities using penalization

methods. Numerical solutions can be found with the help of an iteration process; examples for a penny shaped crack show quite good coincidence of both criteria, but the Griffith criterion predicts a little bit larger propagation of the crack than the Irwin criterion.

OPTIMAL AND MOVING MESHES

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Introduction:

A great deal of effort is currently being put into mesh refinement using mesh subdivision but similar improvements in resolution can often be obtained much more cheaply by making adjustments to the mesh. This symposium is concerned with recent advances in the construction of optimal and moving meshes for problems which exhibit sharp features. It includes the use of Moving Finite Element techniques, equidistribution, and variational methods (plus least squares) to move the mesh, as applied to the solution of partial differential equations on unstructured meshes.

Least Squares Moving Finite Elements:

The Moving Finite Element (MFE) method has achieved a good deal of success in its application to parabolic problems, but when applied to purely hyperbolic PDEs moves nodes with approximately characteristic speeds which clearly renders the method useless for steady-state problems. We describe here a least squares extension of MFE, the so-called "static least squares MFE" method (static LSMFE) for steady-state pure-convection problems which corrects this defect. We consider least squares extensions for both transient and steady-state pure convection problems in 1-D, of which static LSMFE is the most successful, and it remains highly successful in 2-D. The nodes are not swept downstream as in MFE and the grid aligns automatically with the flow, thereby yielding far greater accuracy than from the corresponding fixed node least squares results.

MODELING OF NONLINEAR HYSTERESIS IN ELASTOMERS

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In this talk we present a nonlinear hysteretic model for filled elastomers undergoing simple extension. Computational and experimental results are shown to demonstrate that a nonlinear stress-strain law is adequate to describe the behavior of unfilled or very lightly filled elastomers, whereas hysteresis needs to be incorporated for more highly filled rubber samples. Our constitutive law for filled elastomers makes use of a Boltzmann hysteresis integral, and it can also be interpreted in terms of an internal variable formulation. The corresponding dynamical model is shown to be well-posed. We validate this model by presenting very good agreement between model predictions and experimental data both in the quasi-static and the dynamic case.

FEM FOR MHD

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Variational principles will be presented for some two dimensional magnetohydrodynamic flow problems involving strong transverse magnetic fields. The first principle for the stream function-vorticity formulation incorporates the wall no-slip condition as a natural boundary condition. Numerical results based on isoparametric elements are found via a corrected version of a well known non-symmetric frontal solver. The second principle for duct flows has applications to advection diffusion problems. Numerical solutions found by the non-symmetric frontal solver produce non-oscillatory solutions for Hartmann numbers as large as 1000 in contrast to others in the recent literature. It is found for both formulations that accurate core flows can be found even when the thin Hartmann boundary layers are not accurately resolved.

IMPROVING FINITE ELEMENT METHODS FOR FABRICATED STRUCTURES

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Finite element models of fabricated structures are characterised by many junctions between dissimilar elements (for example axials and panels) and the elements are 'uninformed' in that they approximate the exact structural geometry. Due to these inevitable modelling assumptions, error estimators and indicators are elusive: adaptive refinement is difficult: and load output is the most reliable output form. However, load output is best understood as a 'load distribution indicator' since it is only a representation of the true load distribution and needs appropriate interpretation.

Analysis requirements for helicopter structures include static, dynamic, fatigue and damage tolerance as well as special cases. Also, at higher load levels, non-linear panel buckling behaviour is significant. It is common industrial practice for a single finite element model to have many load cases and the output interpreted to suit the nature of the analysis and the details of the true geometry.

This paper presents current developments at GKN Westland Helicopters Limited. It describes a procedure for finite element methods of fabricated structures that, by simple post-processing and a flexible database accessing program, promotes effective downstream usage of finite element output.

In particular, 'nodal load interpretation' is useful for comparing different elements and presenting finite element concepts to stress engineers. 'Parent element' post-processing techniques reduce the volume of output from fine mesh regions and effectively increase element libraries of proprietary finite element codes. Force extraction and force redistribution distinguish load distribution variations with complementary merits in downstream analysis. FORTRAN prototypes and professional codes with a graphical interface enable tests against EH101 full airframe strain gauge correlation measurements as well as a Lynx rear fuselage and hand worked examples.

FINITE ELEMENT SIMULATION IN ORTHOPAEDY USING MRI

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Abnormality in human joint biomechanics is the main cause of the degenerative disease development, therefore the description and correction of the joint biomechanics is essential for adequate treatment. We present an approach how to obtain the data of a patient and how to use these data subsequently in 3D mathematical models. The Magnetic Resonance Imaging (MRI) of the hip joint is used as a base for 3D simulations. The MRI output has to be transformed into a form readable by our FE software. Two transformators were developed for this purpose. To analyse the model as a contact problem, some further transformations are necessary. A contact is assumed between the femur and the pelvis. We compare the results both from the elastic and from the contact analyses.

NUMERICAL SOLUTION OF FLUID-STRUCTURE INTERACTION USING FINITE ELEMENTS

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We assume viscous incompressible fluid, described by unsteady Navier-Stokes equations and elastic solid, described by Lame equations in a bounded domain of \mathbb{R}^3 . Assume, that fluid and structure have common part of the boundary, interface Γ_I .

First, for the case of small dispacements, when we can neglect the moving boundary of the fluid in time, we consider fixed domain of the fluid and following conditions on the interface Γ_I between the fluid and structure

- 1) all components of the fluid velocity are equal to structural velocity components
- 2) continuity of all components of normal stress vector

Then for the case of Stokes problem we are able to prove an existence result for the coupled problem using Lions-Magenes theory.

Second, we study numerical analysis of the time dependent coupled problem for the case of Navier-Stokes equations and an elastic structure, where both fluid and structure are discretized by finite elements.

After time discretization when coming from time t^n to t^{n+1} for resolution in spatial variables we use domain-decomposition like technique: We start with the solution of the fluid problem for some velocities prescribed on the interface. After that, fluid stress on the interface acting on the structure can be computed. Resolving the problem of an elastic body gives us displacements, velocities and acceleration of the elastic body. New velocities, obtained on the interface, will be, of course, different from the prescribed ones. For the next space iteration we choose a convex combination of old and new velocities on the interface.

For convergence, we check the difference $\|v_f - v_s\|$ in L^2 norm on the interface Γ_I . After the convergence is reached, we can continue with solution in the next time step. Methods of acceleration of this algorithm are discussed and a results of simple numerical example of flow accross a vibrating plate is presented.

Third, for the case, when moving geometry of the fluid domain is considered, we discuss a similar energy-conserving algorithm based on Arbitrary Lagrangian-Eulerian method and ideas described in [P. Le Tallec, J. Mouro, Structures en grands déplacements couplés à des fluides en mouvement, Rapport de recherche No 2961, INRIA, 1996] including an updating strategy of the interface position.

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ADAPTIVITY AND CONTROL OF FINITE ELEMENT METHOD FOR PLATE STRUCTURES

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Our study proposes a strategy for controlling the quality of the Finite Element Analysis of plate structures. It is based on the concept of error in the constitutive relation, and on associated techniques of mesh adaptivity. The aim herein is to guarantee for the user of this method a global accuracy at a minimum computational cost.

This concept of the error in the constitutive relation, which has already been successfully used in many domains (2D-3D elasticity, non-linear analysis, dynamics, etc) [Ladevèze, Accuracy of elastoplastic and dynamic analysis in Accuracy of elastoplastic and dynamic analysis, Ed. J. Wiley, 1986, pp. 181–203] consists of building an admissible displacement-stress field with respect to a reference model. This construction uses both the finite element solution and the problem data. Then, the accuracy of the finite element solution is evaluated with the verification of the constitutive relation by this admissible field.

For plate structures, the main point of the strategy is the construction of a generalised stress and displacement. The two plate models, Kirchhoff-Love and Reissner-Mindlin, can be taken as reference models.

Two methods of building the statically-admissible shear force and bending moment are developed. The first one is a direct extension of the 2D method, using a sub-cutting of the element. The second is more specific to plate problems. Without sub-cutting, the latter method yields a more regular bending moment within the element.

The discretisation of plate structures was performed using the DKT element [Batoz J.-L., A study of 3-node triangular plate bending element, Int. J. of Num. Meth. in Eng. 15, 1980, pp. 1771–1812]. We show, with the help of examples where the exact solutions are known, that the estimators we have developed present a very high level of accuracy. The convergence rate of the calculated error is the same as that of the exact error, and the effectivity index (ratio between calculated error and exact error) is close to 1.

Since these error estimators are known, the techniques of adaptive meshing [Coorevits P., Ladevèze P. and Pelle J.P., An automatic procedure for finite element analysis in 2D elasticity, Comp. Meth. Appl. Mech. Eng. 121, 1995, pp. 91–120] therefore used. These coupled strategies also yield optimal meshes.

**FINITE ELEMENT APPROXIMATION OF A
QUADRATIC EIGENVALUE PROBLEM ARISING IN
DAMPED FLUID-STRUCTURE INTERACTIONS**

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We consider a quadratic eigenvalue problem which arises in the determination of the vibration modes of a fluid-structure system with interface damping. The coupled system consists of an elastic structure containing an acoustic fluid, with a thin layer of a viscoelastic material separating both media.

Displacement variables are used for fluid and solid, whereas the effect of the damping material is modeled by conveniently modifying the interface constraints. This leads to a quadratic variational eigenvalue problem which is discretized by adapting a finite element methodology introduced and analyzed in [1, 2] for undamped elastoacoustic vibrations. It consists of using standard piecewise linear continuous elements for the structure combined with lowest order Raviart-Thomas ones for the fluid.

In the simpler case of a perfectly rigid structure, the spectrum of the continuous problem is thoroughly characterized by following the lines of [4]. Two types of free vibration modes are shown to be present in this model: the standard damped oscillation modes and overdamped ones arising from the modeled behavior of the viscoelastic material.

It is shown that both kind of modes can be reliably computed by the proposed method and that no spurious pollution (typical in other displacement formulations) is introduced. Optimal order error estimates for eigenfunctions and eigenvalues are proved. Further numerical experiments exhibiting the good performance of the method and confirming the theoretical results are reported in [3].

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FINITE ELEMENT METHODS FOR FLUID-STRUCTURE VIBRATION PROBLEMS

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In the first part we recall different formulations of some fluid-structure vibration problems, more precisely, those concerning elastoacoustics and hydroelasticity. These formulations correspond to several possible choices of fields characterizing the motion of the fluid; namely, pressure, pressure/potential, displacements, etc. They can be obtained through linearization of the motion equation in the reference configuration.

Then we discuss advantages and disadvantages of all of them in view of their numerical solution, by writing the weak formulations for their respective spectral problems and analyzing mathematical properties like compactness, symmetry, etc.

In the second part we restrict ourselves to the displacement formulation and give an overview of different finite element discretizations which have been proposed in the literature for its numerical solution. We consider in particular the use of Raviart-Thomas finite elements to approximate the fluid displacement field as proposed in references [1] and [2]. The advantage of this approach with respect to classical Lagrangian finite elements is that no spurious modes are obtained. We prove optimal error estimates both for eigenmodes and eigenfrequencies and show numerical results for some test problems.

Finally, in the case of hydroelasticity under gravity, we compare this methodology to those based on the classical added mass formulation (see for instance [4] and [3]).

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AN APPLICATION OF PARALLEL HIGH PERFORMANCE COMPUTING FOR ANALYSIS OF STRESS FIELDS INDUCED BY MINING

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Mathematical modelling in geomechanics often requires finite element analysis in large 3D domains, modelling of several development stages and treatment of some uncertainty in the input data. These requirements then need the use of high performance computing facilities including parallel multicomputers and corresponding numerical methods.

We describe an example of finite element modelling of stress fields induced by mining which belongs to the above category. The characteristic features of our example are large 3D domain of interest, boundary conditions representing action of surrounding rocks under complicated initial stress state and modelling of several selected stages of mining. The complexity of the modelling is given by repeated use of finite element analysis with nearly four million degrees of freedom and solution of singular problems due to necessity of using pure force boundary conditions at least in one modelling stage.

The computations performed for the described modelling use the displacement decomposition technique which was firstly introduced for constructing incomplete factorization preconditioners by Axelsson and Gustafsson. This technique is used for construction of fixed and variable preconditioners as well as for parallelization of the preconditioned conjugate gradient method. The variable preconditioner is equipped by reorthogonalization of the search directions. Moreover, for the solution of singular problems (nonunique displacements, unique stresses), we propose a stabilization of the conjugate gradient iterations by projection of residuals to the range of the stiffness matrix.

The efficiency of the described numerical methods is demonstrated on the computations performed on the IBM SP multicomputer. Especially, the variable preconditioning is shown to be very efficient with a superlinear speed up in our parallel implementation.

FINITE ELEMENT APPROXIMATION FOR MAXWELL'S EIGENPROBLEM

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The vibration frequencies of the electric field are governed by the following eigenvalue problem derived from the Maxwell's equations:

$$\begin{cases} \underline{\operatorname{curl}}\left(\frac{1}{\mu} \underline{\operatorname{curl}} \underline{u}\right) = \omega^2 \varepsilon \underline{u} & \text{in } \Omega \\ \operatorname{div}(\varepsilon \underline{u}) = 0 & \text{in } \Omega \\ \underline{u} \cdot \underline{t} = 0 & \text{on } \partial\Omega \end{cases} \quad (1)$$

where \underline{u} is the electric field, Ω a polyhedral domain possibly non-convex, $\partial\Omega$ its contour and \underline{t} the counterclockwise oriented tangent versor. The function μ and ε are given, strictly positive and bounded and represent respectively the magnetic permeability and the electric permittivity.

The physical modes satisfy automatically the divergence-free constraint, so that a typical approach in view of the numerical discretization is to drop out the constraint and to discard a posteriori the unphysical modes corresponding to the zero frequency, which are added to the spectrum. However not all the finite element discretizations provide good results in order to easily recognize the physical modes among the computed ones.

Recently in [D. Boffi, P. Fernandes, L. Gastaldi, I. Perugia, Computational models of electromagnetic resonators: analysis of edge element approximation, to appear on SIAM Jour. Numer. Anal.], it has been shown that suitable finite element methods for this approach should also give good results when applied to an eigenproblem in mixed form which is equivalent to the original problem (1). Hence the analysis of the convergence and accuracy properties of a finite element method approximating problem (1) is reduced to the analysis of the convergence and the accuracy properties of such finite element method when applied to the equivalent eigenproblem in mixed form.

We want to describe the features of the analysis of the approximation by finite elements of an eigenproblem in mixed form, starting from the choice of a suitable compact resolvent operator, passing through the individuation of sufficient conditions which ensure the uniform convergence of such operator, which in turn implies the convergence of the spectrum and of the eigenspaces, see also [D. Boffi, F. Brezzi, L. Gastaldi, On the problem of spurious eigenvalues in the approximation of linear elliptic problems in mixed form, to appear on Math. Comp.] and [D. Boffi, F. Brezzi, L. Gastaldi, On the convergence of eigenvalues for mixed formulations, Ann. Scuola Norm. Sup. Pisa Cl. Sci., Vol. XXV, 1997, pp. 131-154] and finally applying the above results to some suitable choice of finite elements, see [D. Boffi, Discrete compactness and Fortin operator for edge elements, submitted to Numer. Math.].

NONSTANDARD FINITE ELEMENTS FOR MAXWELL'S EIGENPROBLEM IN NONCONVEX DOMAINS

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The simplest form of Maxwell's eigenproblem reads as follows:

$$\begin{aligned} & \text{find } (\lambda, \underline{u}) \text{ with } \underline{u} \not\equiv 0 \text{ s.t.} \\ & \left\{ \begin{array}{ll} \underline{\operatorname{curl}} \underline{\operatorname{curl}} \underline{u} = \lambda \underline{u} & \text{in } \Omega \\ \operatorname{div} \underline{u} = 0 & \text{in } \Omega \\ \underline{u} \times \underline{n} = 0 & \text{on } \partial\Omega \end{array} \right. \end{aligned} \quad (1)$$

In the first part of the talk we recall some known finite element methods to approximate (1). Among those we suggest in particular the use of the edge elements (see [3]). It turns out that the edge elements perform well even in presence of singularities like the ones produced by nonconvex domains. In particular a new *hp*-adaptive edge formulation seems to be a good solution (see [5]). Implementation issues are analyzed in [1].

In the second part we discuss about the following penalty variational formulation of (1).

$$\begin{aligned} & \text{find } (\lambda, \underline{u}) \text{ with } \underline{u} \not\equiv 0 \text{ s.t.} \\ & (\underline{\operatorname{curl}} \underline{u}, \underline{\operatorname{curl}} \underline{v}) + s(\operatorname{div} \underline{u}, \operatorname{div} \underline{v}) = \lambda(\underline{u}, \underline{v}) \quad \forall \underline{v} \end{aligned} \quad (2)$$

It has been pointed out in [4] that finite element spaces to approximate (2) have to be chosen very carefully. In particular no standard finite element (even with local refinement) can give satisfactory results in presence of reentrant corners/edges. We adapt a nonstandard finite element scheme proposed in [2] (see also [6]) for a different problem. Numerical experiments and a partial numerical analysis is provided.

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AN ACCURATE FINITE ELEMENT SOLUTION OF THE BIHARMONIC EIGENPROBLEM

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We consider the accurate numerical approximation of the spectral properties of the biharmonic operator on various domains in two dimensions. A number of analytic results concerning the eigenfunctions of this operator are briefly summarized and their implications for numerical approximation are discussed. In particular, the asymptotic behaviour of the least eigenfunction is studied since it is known that it has an unbounded number of oscillations when approaching sufficiently small corners on domain boundaries. We demonstrate that a number of these oscillations may be accurately computed using an unstructured finite element solver. As a starting point in our computations we adopted the mixed finite element method for the biharmonic problem due to Ciarlet and Raviart which enabled us to solve the problem using C_0 elements. A key to obtaining accurate results in the vicinity of a corner is to use appropriate triangulation which involves unstructured and highly non-uniform meshes. Because high accuracy in the solution of the resulting linear system is needed, we adopt the direct method for its solution. We present a number of numerical results obtained on a variety of domains, such as the unit square, a family of circular sector domains, and another family of symmetric non-convex domains referred to as the dumb-bell shape domains. For the circular sector domains the oscillatory behaviour is studied as a function of internal angle, and for the dumb-bell shape domains the parity of the least eigenfunction is investigated. At the end we give some comments on the quality of the finite element method for this problem by comparing it with some highly accurate spectral methods.

AN A POSTERIORI ERROR ESTIMATE FOR THE STOKES PROBLEM IN A POLYGONAL DOMAIN

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1. The Stokes Problem.

Let $\Omega \subset R^2$ be a polygonal domain. On $(H_0^1(\Omega)^2 \times L_0^2(\Omega))^2$ we define the bilinear form $\mathcal{A}(\{v, p\}, \{v^*, p^*\}) = \nu(\nabla v, \nabla v^*) - (p, \operatorname{div} v^*) + (p^*, \operatorname{div} v)$, where $(.,.)$ means the scalar product in L^2 , v is the velocity vector, p is the pressure, $\{v, p\}$ denotes the vector $\{v_x, v_y, p\}$, $\nu > 0$ is the viscosity. Let $f \in L^2(\Omega)^2$. The Stokes problem then consists in finding $\{v, p\} \in H^1(\Omega)^2 \times L_0^2(\Omega)$ such that

$$\mathcal{A}(\{v, p\}, \{v^*, p^*\}) = (f, v^*) \quad \forall \{v^*, p^*\} \in H_0^1(\Omega)^2 \times L_0^2(\Omega). \quad (1)$$

2. Finite Element Approximation.

Let \mathcal{T}_h be regular and quasiuniform triangulations of Ω . Let X^h, M^h be the finite element spaces of Hood-Taylor elements. The finite element approximation of the Stokes problem consists in finding $\{v_h, p_h\} \in X^h \times M^h$ such that

$$\mathcal{A}(\{v_h, p_h\}, \{v_h^*, p_h^*\}) = (f, v_h^*) \quad \forall \{v_h^*, p_h^*\} \in X^h \times M^h. \quad (2)$$

3. A Posteriori Error Estimate.

We follow the idea of [Eriksson, K., Estep, D., Hansbo, P., Johnson, C., Introduction to adaptive methods for differential equations. *Acta Numerica*, CUP, 1995, 105–158] who proved the a posteriori error estimate for the Poisson equation.

We define the residual components by the relation

$$R_1\{v_h, p_h\} = f + \nu \Delta v_h - \nabla p_h, \quad R_2\{v_h, p_h\} = \operatorname{div} v_h.$$

Next we study the properties of the errors $e_v = v - v_h$, $e_p = p - p_h$, where $\{v, p\}$ is the exact solution of (1), $\{v_h, p_h\}$ is the approximate solution defined in (2). We prove the following a posteriori error estimate

$$\begin{aligned} \|e_v\|_1 + \|e_p\|_0 &\leq 2 C_P C_I C_R \sum_{K \in \mathcal{T}_h} \left[h_K \|R_1\{v_h, p_h\}\|_{0,K} + \right. \\ &\quad \left. + \|R_2\{v_h, p_h\}\|_{0,K} + h_K^{\frac{1}{2}} \sum_{l \in \partial K} \frac{1}{2} \nu \left\| \left[\left[\frac{\partial v_h}{\partial n} \right] \right]_l \right\|_{0,l} \right], \end{aligned} \quad (3)$$

where C_P , C_R , C_I are positive constants, and where we denote $\llbracket \left[\frac{\partial v_h}{\partial n} \right] \rrbracket_l = \frac{\partial v_h}{\partial n} \Big|_{l+} - \frac{\partial v_h}{\partial n} \Big|_{l-}$, the jump of the normal derivative along the common side l of two adjacent triangles.

Let us note that for convex domains stronger regularity applies to the Stokes problem, and better a posteriori error estimate is expected. For nonconvex domains with corners we do not obtain so strong regularity, cf. e.g. [Burda, P., On the F.E.M. for the Navier-Stokes equations in domains with corner singularities, in Finite Element Methods, Ed. by M. Křížek et al., Marcel Dekker, New York, 1998, pp. 41-52], but still the a posteriori error estimate should be better than in (3).

We compare these results to a posteriori error estimates for the Poisson equation both on the convex and nonconvex polygon. In the end we give some numerical results.

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LARGE TIME-STEP OPERATOR SPLITTING METHODS FOR NONLINEAR STRONGLY DEGENERATE CONVECTION- DIFFUSION EQUATIONS AND APPLICATIONS TO THE THEORY OF SEDIMENTATION-CONSOLIDATION PROCESSES

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In one space dimension, the phenomenological theory of sedimentation-consolidation processes reduces to an initial-boundary value problem for a second-order nonlinear strongly degenerate convection-diffusion equation. Due to the mixed hyperbolic-parabolic nature of the model, its solutions are in general discontinuous and difficulties arise if one tries to construct these solutions by classical numerical methods. In this paper we present and elaborate on numerical methods that can be used to correctly simulate this model, i.e., conservative methods satisfying a discrete entropy principle. Included in our discussion are finite difference methods and methods based on operator splitting. These methods are employed to simulate the settling of flocculated suspensions.

VALUATION OF FINANCIAL OPTIONS WITH PROBABILISTIC FINITE ELEMENTS

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The value of an option or option-like contingent claim depends on parameters such as the instantaneous riskfree interest rate and the volatility of the underlying assets which are estimated from historical data and thus are subject to statistical errors. The probabilistic finite element method (PFEM) provides an estimate of the standard error of the option value in terms of the standard errors of the estimated model parameters. It also gives the sensitivities to the model parameters and a second order correction to the option value that would be obtained using numerical methods which ignore the errors in data. To obtain the effect of errors in the parameters, element interest rate stiffness and volatility stiffness matrices are computed separately and assembled separately. Examples are presented on optimal capital structure for firms, options on the minimum or maximum of several assets, comparison of options on futures and options on the spot, and tests of option pricing models.

The Brennan-Schwartz result on the existence of an optimal capital structure in the absence of personal income taxes and bankruptcy costs is valid also if the volatility is estimated from historical data.

In the finite element model for an option on the minimum or maximum of several assets, there are elements of all dimensions up to the number of assets. Unnecessarily large global matrices are avoided by taking into account the skeletal structure of the model. It is shown that the value of right to early exercise increases with the number of underlying assets and the additional value is estimated. There will be some Euro-related options belonging to this class during the transition period.

The distribution of second order corrections to the values of options on futures and options on the spot and the standard errors of the calculated values is of interest to both investors and traders, and in designing tests of market efficiency or option pricing models. As an example, American puts are considered with an instantaneous riskfree interest rate of 0.15 per annum and instantaneous variance rates ranging from 0.04 to 0.25, with a coefficient of variation of 25% which corresponds to one month asset returns data in the case of volatility. Maximum standard errors occur at the money, about 25% of the option value, futures-spot difference being about 2.5%. Errors for futures are larger than those for the spot in the money, smaller out of the money. The maximum difference is 5% away from the money. It occurs at medium variance in the money, at low variance near in the money, and at high variance rates out of the money. The second order corrections for futures are smaller than those for the spot at low variance rates, larger at high variances. The corrections are positive for low variance, negative at high variance rates. The size grows to 1.5% with variance and maturity. The signs of corrections are the same for spot European calls which have been subjected to extensive tests and agree with the biases found by Black and Scholes, suggesting that second order corrections due to volatility estimation errors may explain at least in part those observed biases.

**A FAST TWO-GRID AN FINITE SECTION METHOD
FOR AN ACOUSTIC SCATTERING PROBLEM
IN THE HALF-PLANE**

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We consider the solvability and numerical treatment of a class of second kind integral equations on the real line of the form

$$\phi(s) = \psi(s) + \int_{-\infty}^{+\infty} \kappa(s-t)z(t)\phi(t)dt, \quad s \in \mathbb{R},$$

(abbreviated $\phi = \psi + K_z\phi$) in which $\kappa \in L^1(\mathbb{R})$, $z \in L^\infty(\mathbb{R})$, $\psi \in BC(\mathbb{R})$ are assumed known and $\phi \in BC(\mathbb{R})$ is to be determined. We first recall conditions on a set $W \subset L^\infty(\mathbb{R})$ which ensure that if $I - K_z$ is injective (on $BC(\mathbb{R})$) for all $z \in W$ then $I - K_z$ is surjective for all $z \in W$ and the inverse operators $(I - K_z)^{-1}$ are uniformly bounded in z . We also discuss conditions which ensure that the finite section method (truncation of the range of integration to $[-A, A]$) is stable, uniformly in z .

We then discuss solvability in the weighted space $BC_w(\mathbb{R}) := \{\psi \in BC(\mathbb{R}) | w\psi \in BC(\mathbb{R})\}$, for classes of weight functions w (including $w(s) = (1 + |s|)^p$, with $p \geq 0$). We show that, if some mild conditions on w and κ are satisfied, then the spectrum and essential spectrum of $I - K_z$ is the same on $BC(\mathbb{R})$ as on $BC_w(\mathbb{R})$. These results on solvability in weighted spaces enable us to obtain sharp error estimates for the finite section method.

We next discuss and analyse a numerical method for the finite section equation on $[-A, A]$, a semi-discrete collocation method on a uniform grid with an iterative solver based on a two-grid iteration and an approximation of the full coarse grid matrix by a banded matrix: the uniform grid and the discretisation adopted enable the matrix-vector multiply to be carried out efficiently using the FFT.

As an application we consider an acoustic scattering problem in the half-plane with a Robin or impedance boundary condition which we formulate as a boundary integral equation of the class studied. Our final result is that provided z (the boundary impedance in the application) takes values in a compact convex subset Q in the complex plane then the difference between $\phi(s)$ and its finite section approximation computed numerically using the iterative scheme proposed is $\leq C_1 kh \log(1/kh) + C_2(1 - \theta)^{-1/2} A^{-1/2}$ in the interval $[-\theta A, \theta A]$ ($\theta < 1$), for kh sufficiently small, where k is the wavenumber and h the mesh-size. Moreover this numerical approximation can be computed in $\leq C_3 N \log N$ operations, where $N = 2A/h$ is the number of degrees of freedom. An attractive feature of the analysis is that the values of the constants C_j , $j = 1, 2, 3$, depend only on the set Q .

A MODEL FOR GROUTED ROCKBOLTS, USING A BEAM FORMULATION

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A one-dimensional finite element formulation is presented, which can be used to model individual steel rockbolts, fully-grouted to the surrounding rock, and either passive or pre-tensioned.

The new element is based on the distinct rockbolt element developed in [Ö. Aydan, Ph.D. Thesis, Nagoya, 1989] for use in 3D meshes, which consists of a linear (2-noded) bar representing the steel bolt, coupled with six nodes which attach to the surrounding rock elements. The grout behaviour is modelled by constitutive laws for normal and shear forces defining interactions between these two sets of nodes.

Adaptations of this element for use in 2D meshes, by Aydan and others — for example in [M. Marenč, Ph.D. Thesis, Innsbruck, 1991] — have maintained the piecewise-linear bar representation of the bolt, with special ‘bolt-crossing-joint’ elements needed at locations where the bolt crosses a joint in the rock mass. The one-dimensional element proposed here contains six nodes, of which three are for attachment to the rock mesh (discretised with ‘serendipity’ quadrilateral elements). Combined with this, two different models for the three-noded bolt have been tested: a quadratic bar formulation which transmits normal and shear forces but not bending moments, and a beam formulation which uses Hermite quartic basis functions. The element formulation also incorporates large-displacement theory.

In tests on a wedge stability problem, with a mesh combining continuum, joint and bolt elements, it is shown that the new element with a beam formulation for the bolt is capable of predicting realistic deformation of the bolt and support of the wedge.

A POSTERIORI ERROR ESTIMATES FOR SPECTRAL ELEMENT SOLUTIONS TO VISCOELASTIC FLOW PROBLEMS

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The present work is an attempt to provide some theoretical undergirding to the question of appropriate error estimators for numerical solutions to viscoelastic flow problems. The main result is a demonstration, under mild assumptions, that for numerical simulations of flows of a slightly elastic Oldroyd B fluid the square of the norm proposed by Warichet and Legat [2, 3] for our estimated errors is equivalent to the sum of the squares of norms of the exact error for the velocity, pressure and stress. In proving the result inspiration has been drawn from arguments used by, for example, Oden et al. [1], in their work on a posteriori error estimates for numerical solutions to the Navier-Stokes equations. We also show uniqueness and existence for the estimated errors. At this stage we do not have any theoretical results for an element residual method so that the weak error equations are approximated directly, rather than on an element by element basis, and we use a spectral element method to do this. As an illustration of the use of our error estimates we describe a spectral element method for flow of an Oldroyd B fluid past a sphere in a tube. Numerical results are presented to show how the approximate error and the ‘exact’ error obtained by calculating the difference between the numerical solution and a reference calculation decrease with mesh refinement.

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MODELLING OF UNDERGROUND EXCAVATION IN TWO-PHASE MEDIA

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A proper evaluation of the stress distribution and of the time dependent deformation around tunnels driven into saturated soil/rock deposits should consider two main sources of non-linearity.

The first one has a geometrical nature and is introduced by the advancing of the excavation and by the installation of the temporary and permanent supports.

The second one is related to various phenomena that govern the mechanical behaviour of the spoil/rock mass, among which the following can be mentioned:

- a) The dissipation of the excess pore pressure in the medium surrounding the tunnel caused by the excavation process.
- b) The elasto-plastic soil/rock behaviour induced by the stress concentration in the vicinity of the opening.
- c) The development of time-dependent (or creep) deformation.
- d) The possible attainment of partially saturated conditions.
- e) The strain localization that can occur in the presence of softening behaviour of the materials.

Here, the main aspects are summarized of some computational procedures adopted for modeling the above effects. Reference is made to a series of simple cases in view of the application to actual engineering problems.

The analysis of two-phase problems is cast into the framework of the so-called "coupled approach" for consolidation, explicitly considering the interaction between fluid and solid phases. The discussion is confined to the static regime in plane strain conditions, even though the extension to the three dimensional case does not present particular difficulties.

The following computational aspects are discussed in particular:

- The numerical simulation of the excavation process in two-phase media.
- Some details of the elasto-plastic analysis based on Mohr-Coulomb yield criterion and, finally,
- A simple approach for modeling the occurrence of partially saturated conditions around the tunnel.

PARALLEL COMPUTATION OF FLOW IN HETEROGENEOUS MEDIA MODELLED BY MIXED FINITE ELEMENTS

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In this talk we describe a fast parallel method for solving highly ill-conditioned saddle-point systems arising from simulations of stochastic PDEs which model flow in heterogeneous media using mixed finite elements. Each realisation of these stochastic PDEs requires the solution of the linear first-order velocity-pressure system for groundwater flow comprising Darcy's law coupled with an incompressibility constraint. The chief numerical difficulty is that the hydraulic conductivity takes a different value on each element, and may vary by many orders of magnitude from element to element, especially when the statistical model has a large variance and a small correlation length. We solve these problems by first reducing the saddle-point formulation to a symmetric positive definite problem using a suitable basis for the space of divergence-free velocities. The result is a bordered system that is about a fifth of the size of the original indefinite system, and whose main block is equivalent to a standard linear finite element discretisation of a related 2nd-order elliptic problem. The theory of preconditioning of this block is well understood, and we use conjugate gradients preconditioned with an algebraically determined additive Schwarz domain decomposition preconditioner to invert it. The result is a solver which exhibits a good degree of robustness with respect to the mesh size as well as to the variance and to physically relevant values of the correlation length of the underlying conductivity field. Numerical experiments on problems with up to 10^6 degrees of freedom have exhibited very high levels of parallel efficiency on an IBM SP/2.

The domain decomposition solver
(DOUG, <http://www.maths.bath.ac.uk/~parsoft>)
is not special to this application and can be applied on general parallel architectures to linear systems arising from 2D or 3D finite element discretisations.

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POSTPROCESSING OF HIGH-ORDER ACCURATE GALERKIN METHODS IN LOCALLY TRANSLATION INVARIANT MESHES

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We show that when Galerkin methods for convection, like the standard Galerkin method, the Discontinuous Galerkin method, or the streamline diffusion method, are defined in locally translation invariant meshes, it is possible to postprocess the approximate solution and obtain a much better approximation- if the exact solution is smooth enough. The postprocessing is a convolution with a kernel of support of order h and hence is very cheap; also, it has to be done only once at the end of the computation. Thus, the postprocessed approximation of the DG method is proven to be order $2k+1$ in L^2 when polynomials of order k are used. This must be contrasted with the classical order of convergence in L^2 , namely, $k+1/2$.

This is joint work with M. Luskin, C.-W. Shu, and E. Suli.

BOUNDARY CONDITIONS AND LAYER TECHNIQUE FOR THE SIMULATION OF ELECTROMAGNETIC WAVES ABOVE A LOSSY MEDIUM

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Two innovative techniques for the simulation of the effect of a lossy dielectric half-space $z > 0$ are derived and analysed. The first is an adapted impedance surface condition imposed at the interface to replace the dielectric medium. This condition is written as follows:

$$\left(\epsilon_s \mu_s \frac{\partial^2}{\partial t^2} + \sigma_s \mu_s \frac{\partial}{\partial t} + \vec{\text{curl}}_\Gamma(\text{curl}_\Gamma) \right) \vec{E}_t - \epsilon_s \mu_s Z_a \frac{\partial^2}{\partial t^2} \vec{H}_\tau = 0 \quad \text{on } z = 0 \quad (1)$$
$$\vec{E}_t = \hat{z} \wedge (\vec{E} \wedge \hat{z}), \quad \vec{H}_\tau = \vec{H} \wedge \hat{z}$$

where Z_a is a well chosen differential operator which operates on functions of the variables (x, y, t) .

This condition, when coupled with Maxwell's equations yields a stable system which can be written in a variational form. It allows us to take into account both the polarization and the angle of incidence of the out-going waves.

The second technique is a generalization of the Bérenger perfectly matched layers: the dielectric is now replaced by a short length layer in which the waves are governed by a modification of Maxwell's equations. The idea consists in substituting for the real dielectric an artificial model, that provides the same reflection coefficient as does the real dielectric while enforcing the attenuation inside the layer. Let us remark that this is the case for Bérenger's PMLs when the dielectric is a trivial dielectric, i.e. a free space, and consequently the reflection coefficients are zero. Our purpose is then to generalize the PML's to the case of a non-trivial dielectric. The solution we propose

consists in substituting to the Maxwell system of equations the following system of 12 equations with 12 unknowns

$$\left\{ \begin{array}{l} \epsilon \frac{\partial E_z}{\partial t} + \sigma E_z = \frac{\partial (H_{yz} + H_{yx})}{\partial x} - \frac{\partial (H_{xy} + H_{xz})}{\partial y}, \quad \epsilon \frac{\partial E_{yz}}{\partial t} + \sigma E_{yz} = \epsilon \frac{\partial \Psi_y}{\partial t}, \\ \epsilon \frac{\partial E_{yx}}{\partial t} + \sigma E_{yx} = - \frac{\partial H_z}{\partial x}, \quad \epsilon \frac{\partial \Psi_y}{\partial t} + \sigma_z \Psi_y = \frac{\partial (H_{xy} + H_{xz})}{\partial z} \\ \epsilon \frac{\partial E_{xy}}{\partial t} + \sigma E_{xy} = \frac{\partial H_z}{\partial y}, \quad \epsilon \frac{\partial E_{xz}}{\partial t} + \sigma E_{xz} = \epsilon \frac{\partial \Psi_x}{\partial t}, \quad \epsilon \frac{\partial \Psi_x}{\partial t} + \sigma_z \Psi_x = - \frac{\partial (H_{yz} + H_{yx})}{\partial z} \\ \mu \frac{\partial H_z}{\partial t} = \frac{\partial (E_{xy} + E_{xz})}{\partial y} - \frac{\partial (E_{yx} + E_{yz})}{\partial x}, \quad \mu \frac{\partial H_{yx}}{\partial t} = \frac{\partial E_z}{\partial x}, \quad \mu \frac{\partial H_{xy}}{\partial t} = - \frac{\partial E_z}{\partial y} \\ \mu \frac{\partial H_{yz}}{\partial t} + \sigma_z^* H_{yz} = - \frac{\partial (E_{xy} + E_{xz})}{\partial z}, \quad \mu \frac{\partial H_{xz}}{\partial t} + \sigma_z^* H_{xz} = \frac{\partial (E_{yz} + E_{yx})}{\partial z} \end{array} \right. \quad (2)$$

where

$$(\epsilon, \mu, \sigma, \sigma_z, \sigma_z^*) = \begin{cases} (\epsilon_0, \mu_0, 0, 0, 0) & \text{if } z < 0 \\ (\epsilon_s, \mu_s, \sigma_s, \epsilon_s \sigma^*, \mu_s \sigma^*) & \text{if } 0 < z < \delta \end{cases} \quad (3)$$

and σ^* , a positive function of z , can be interpreted as an artificial damping factor.

ERROR ESTIMATOR FOR FINITE ELEMENT ANALYSES OF UNILATERAL CONTACT PROBLEM

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The numerical simulation of contact problems is more often carried out by finite element methods. For the user, one important aspect is obviously to evaluate the discretization errors due to the use of this type of approximation. From the point of view of mathematics, a unilateral contact problem corresponds to a variational inequality. The convergence of the associated finite element methods has been studied by numerous authors on the basis of a priori error estimators.

However, these a priori error estimations do not allow us to quantify the discretization errors. This quantification requires the definition of a posteriori error estimations. For linear problems, various research efforts have been performed: estimators based on the residual of the equilibrium equations, estimators using the smoothing of finite element stresses and estimators based on the concept of error in the constitutive relation. For non-linear problems, and especially for the non-linearity of contact, the work available is much less abundant. We can however cite reference [Wriggers P., Scherf O. and Cartensen C., Adaptive techniques for the contact of elastic bodies in Recent developments in finite element analysis, eds. Hughes, Onate, Zienkiewicz, 1994, pp. 78-86] which, based on a penalty method, transforms the variational inequality into a variational equality that allows, within the classical framework, building an estimator based on the residuals. Nevertheless, this estimator explicitly uses the penalty parameter, which does represent a drawback.

We propose, for unilateral contact problems without friction between elastic bodies under small perturbations, an error measure based on the concept of error in the constitutive relation. This error measure can be used for the classical numerical techniques for treatment of the non-interpenetration condition. The development of an error measure in the constitutive relation relies on a classification of the kinematic conditions, equilibrium equations and constitutive relations. In the case of contact, in order to establish this classification, we consider as in [Ladevèze P., Nonlinear computational structural mechanics, New approaches and non-incremental methods of calculation, Springer, 1998] the contact zone as a mechanical entity with its own variables and its own constitutive relations. The quality of an approximate admissible solution which, by definition, satisfies the kinematic conditions and equilibrium equations is evaluated by the manner in which the constitutive relations are satisfied. A link between the error measure in the constitutive relation and the classical errors in the solution is established. For these types of problems, such an approach can be considered as an extension of Prager-Synge's theorem [Prager W. and Synge J.L., Approximations in elasticity based on the concept of function space, Quart. Appl. Math. 5, 1947, pp. 261-269] in elasticity.

Examples of the use of the error estimator as well as examples of adaptive computations are shown.

CRACK AND SCREEN ASYMPTOTICS

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We consider general Agmon-Douglis-Nirenberg elliptic systems with smooth coefficients complemented by the same set of boundary conditions on both sides of a crack or a screen. We investigate the singular functions appearing in the vertex asymptotics at the crack tip and in the edge expansion along the screen. In each geometry (crack or screen) are associated local polar coordinates (r, θ) . We prove that the polar parts of the singular functions have the form $r^{\frac{1}{2}+k}\varphi(\theta)$ with $k \geq 0$ integer, with the possible exception of a finite number of singularities of the form $r^k \log r \varphi(\theta)$: thus the singularity exponents do not depend on the operator and, moreover, most of the logarithmic shadow terms predicted by the general theory do not appear in these situations.

INFINITE ELEMENT METHODS FOR ELASTO-ACOUSTICS: IMPLEMENTATION ASPECTS AND COMPUTATIONAL PERFORMANCES

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Various numerical techniques are available for handling unbounded acoustic domains in a finite element context. The paper focuses on infinite element methods for both steady state harmonic and transient acoustic wave propagation problems governed by the linear wave equation. Both conjugated and unconjugated infinite element formulations are studied. The common roots of both formulations are highlighted (derivation of suitable multipole expansions in various coordinate systems, definition of appropriate functional settings, selection of related variational statements). Implementation aspects are detailed for axi-symmetric and three-dimensional problems. This includes the definition of test and trial functions, the formulation of element matrices and the handling of numerical integration issues. Numerical applications are presented for radiation and scattering problems. Various geometries (spheres, cylinders, plates) are treated in order to demonstrate the convergence of presented methods and to highlight their computational performances. Extensions to other wave propagation problems (convected acoustic wave equation, elasto-dynamic problem) are also outlined.

FEM APPLICATION FOR PREDICTING CHARACTERISTICS OF LINEAR ACTUATOR

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Experience and exploring the linear AC and DC actuators confirm the necessity of computation characteristics, especially the force distribution, as the step preceding their optimal design. The paper expresses an approach to electro-magneto-mechanical coupling in the process of electro-mechanical energy conversion in low-voltage linear actuators in order to obtain the dynamic force characteristics. The computation of dynamic force is based upon FEM application, using magnetic coenergy concept associated with virtual work method and simulated by step displacement of the armature from the fully open through the closed position. The magnetic coenergy will be numerically computed through the flux-linkage approach. The magnetic field distribution will be obtained by applying the Finite Element Method in 3D-domain of the actuator.

The aim of the process of optimal designing of an electromagnetic low-voltage linear actuator is focussed towards the determination of the main design factors such as: dimensions of electric and magnetic circuit(s), characteristics of used materials and

mechanical parameters - springs for opening the armature as well as the contact springs. All of these parameters are taken into account for obtaining the target function - *attractive force* that provides reliable switching in and switching out of the actuator. Many authors treat the problem of force calculation in low-voltage AC linear actuators. In the most number of cases, the force acting on the armature is calculated by different methods, but there is an obvious lack of computations of the forces during switching-in transient period, i.e. implementing the time variation of applied voltage and obtaining dynamic force characteristics.

In the paper will be presented a methodology for predicting characteristics of an actuator, based on the FEM-3D application. The numerical computation of electromagnetic field distribution is carried out by the Finite Element Method (FEM) in the 3D domain and combined with the virtual work principle leads to the most reliable analysis. As the object of investigation, in the paper a 220V AC actuator will be considered. The air gap in the middle core at fully open position is 4.5 mm and at closed position is 0.5 mm, for elimination the remanency.

Application of FEM consists of three main stages: pre-processing, processing and post processing. The geometry of the device allows generation of regular mesh consisting of brick main elements (macros) and their slaves. The slaves are defined by displacement and rotation of the macros. The desired mesh density is controlled by subdividing the macros and their slaves. The required refined mesh density is performed in the region around and in the air gap. The final mesh is obtained by breaking the bricks in triangular prisms. When the linear actuator is analysed, the displacement of yoke affects the geometry, what means that the new mesh generation is to be done at any new position, so there is necessity of automation of this process. This fact leads to special implementation of Finite Element Method in order to simulate the linear movement and improve the automatic mesh generating when implementing the virtual work principle.

Computations continue in the processing stage, enabling the view and the representation of the magnetic field distribution of the actuator, under different loading and displacement conditions. The post processing stage concerns with calculations of electromagnetic and electromechanical characteristics. The force distribution, as an essential matter of analysis, is computed on the basis of magnetic coenergy concept at constant current. The magnetic coenergy is computed numerically by integrating the magnetic flux linkage with respect to the current. Finally, the numerically obtained results will be experimentally confirmed.

**SOLUTION OF PARABOLIC EQUATIONS BY BACKWARD
EULER-MIXED FINITE ELEMENT METHODS ON A
DYNAMICALLY CHANGING MESH**

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We develop and analyze methods based on combining the lowest-order mixed finite element method with backward Euler time discretization for the solution of diffusion problems on dynamically changing meshes. The methods developed are shown to preserve the optimal order error estimates that are well-known for static meshes. The novel aspect of the scheme is the construction of a linear approximation to the solution, which is used in projecting the solution from one mesh to another. Extensions to advection-diffusion equations are discussed, where the advection is handled by upwinding. Numerical results validating the theory are also presented.

This work is joint with Robert Kirby.

FINITE/INFINITE SIMULATIONS FOR MAXWELL'S EQUATIONS

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The paper describes theory and a 2D implementation of the infinite element for steady-state Maxwell's equations [2, 1]. The element is compatible with the hp FE element discretizations for Maxwell's equations in bounded domains reported in [3, 5, 4].

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FINITE ELEMENT APPROXIMATION OF A COUPLING EIGENVALUE PROBLEM IN 2D

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Let Ω be a composite structure in 2D, consisting of two overlapping rectangles Ω_1 and Ω_2 , with respective boundaries $\partial\Omega_1$ and $\partial\Omega_2$. Let moreover Γ_i be a part of $\partial\Omega_i$, consisting of an integer number of sides of Ω_i , such that Γ_i does not intersect with $\partial(\Omega_1 \cap \Omega_2)$, $i = 1, 2$.

We then consider the following variational eigenvalue problem (EVP):

$$\text{Find } [\lambda, u] \in R : a(u, v) = \lambda(u, v) \quad \forall v \in V,$$

where

$$V = \left\{ (v_1, v_2) \mid v_i \in H^1(\Omega_i), v_i = 0 \text{ on } \Gamma_i, i = 1, 2 \text{ and } \int_{\Omega_1 \cap \Omega_2} (v_1 - v_2) dx = 0 \right\}, \quad (1)$$

and

$$a(u, v) = \sum_{i=1}^2 \int_{\Omega_i} \left(\sum_{l,m=1}^2 a_{lm}^{(i)} \frac{\partial u_i}{\partial x_l} \frac{\partial v_i}{\partial x_m} + a_0^{(i)} u_i v_i \right) dx, \quad (u, v) = \sum_{i=1}^2 \int_{\Omega_i} u_i v_i dx.$$

This variational EVP is shown to be formally equivalent with the following differential EVP:

Find $\lambda \in R$ and functions $u_i \in H^2(\Omega_i)$, $i = 1, 2$ which obey, in a weak sense, the differential equations

$$L^{(i)} = \lambda u_i \text{ on } \Omega_i \setminus \overline{\Omega_j}, \quad i = 1, 2, \quad j \neq i, \quad L^{(i)} + F(u) = \lambda u_i \text{ on } \Omega_1 \cap \Omega_2, \quad i = 1, 2$$

accompanied of the boundary conditions

$$u_i = 0 \text{ on } \Gamma_i, \quad i = 1, 2, \quad \frac{\partial u_i}{\partial \nu_a^i} = 0, \text{ on } \partial\Omega_i \setminus \Gamma_i, \quad i = 1, 2,$$

where

$$L^{(i)} \equiv - \sum_{l,m=1}^2 \frac{\partial}{\partial x_m} \left(a_{lm}^{(i)} \frac{\partial}{\partial x_l} \right) + a_0^{(i)},$$

and

$$F(u) = (2 \text{ meas } (\Omega_1 \cap \Omega_2))^{-1} \left[\int_{\partial(\Omega_1 \cap \Omega_2)} \left(\frac{\partial u_1}{\partial \nu_a^1} - \frac{\partial u_2}{\partial \nu_a^2} \right) ds + \int_{\Omega_1 \cap \Omega_2} (a_0^{(1)} u_1 - a_0^{(2)} u_2) dx \right].$$

Such an EVP may arise in the context of heat transfer problems, as has been argued in [F.A. Mehmeti and S. Nicaise, Nonlinear interaction problems, Nonlinear

Analysis, Theory, Methods and Applications, Vol. 20, no.1, 1993, pp.27-61] for a related boundary value problem in 1D.

First of all the variational EVP is shown to fit into a general framework of abstract EVPs for bilinear forms in Hilbert spaces, assuring the existence of exact eigenpairs with suitable properties. Next, we set up finite element methods without and with numerical quadrature. We discuss the error analysis involved, which, due to the coupling condition incorporated in (1), depends heavily upon the introduction and error estimation of a suitably modified (vector valued) piecewise Lagrange interpolant on the FE-mesh.

ON HIGH-ORDER FINITE ELEMENT MODELING OF STIFFENED SHELLS FOR STRUCTURAL ACOUSTICS

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Geometric and higher order finite element modeling of three-dimensional stiffened shell structures for interior and exterior structural acoustics analysis presents many challenges which include:

1. dealing with non-manifold geometries,
2. accurate and valid curvilinear geometric mapping, and
3. discretization of unknown pressure and displacement fields satisfying appropriate continuity requirements.

This presentation will discuss the specification and automated creation of variable-order finite element discretization of the pressure and displacement fields such displacements field is C^0 across the shell junctions and the pressure field is discontinuous across shell surfaces that define the stiffeners (ribs and stringers). Independent specification of the in-plane and through-the-thickness interpolation degrees for the displacement field lead to non-conforming finite element spaces along the shell junctions. Enforcement of appropriate continuity of the displacement field in these cases is based on the following ideas:

1. specification of interpolation degree to individual mesh topological entities, and
2. using mesh topological adjacency information to determine mesh entities along which the pressure field should be discontinuous.
3. use of so-called mortar spaces to “glue” the non-conforming approximations of the displacement field along the junction.

Three-dimensional examples are presented to show the use of the scheme in solving interior and exterior acoustics problems of interest to the navy and aircraft industry.

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USE OF 3D ELEMENTS FOR AN ANALYSIS OF COMPOSITE STRUCTURES

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In this paper we deal with a non-linear behaviour of non-homogeneous composite (especially reinforced concrete) structures loaded by both short-time surface loads and short-time thermal loads. An approach of the analysis using a 3D element (tetrahedron denoted by T48) with an approximation of the displacements, which enables their changes in an element according to the topical stress-strain state is presented. This element uses completely 48 degrees of freedom as follows: - displacements u, v, w and their derivatives in the nodes of tetrahedron (48 degrees). A sufficient approximation of the stress-strain diagram is one of the most important tasks in a non-linear analysis of the materials. We use the same approximation functions as for displacements for the change of moduli of elasticity in the volume of an element according to the topical stress-strain state. A step-by-step procedure for solving the non-linear problem is presented. We divide the total load to a certain number of the increases and in each step of the analysis we precise the matrices of the moduli of elasticity in all points of the element. To derive the topical matrix of the moduli of elasticity in a nodal point of the element we use the certain state of the strain in this node resulting from the previous step of the analysis. We calculate the principal strains in a nodal point, then using the principal strains in previous and topical step we state three "principal" moduli of elasticity along the directions of the principal strains from the certain stress-strain diagram. As a result the matrix of the moduli of elasticity as well as the stiffness matrix change from the step to step according to the certain stress-strain state in a point of the element.

In many engineering problems the stress and strain caused by the thermal loads play an important role by the design of structures. A knowledge of the temperature distribution, both steady and unsteady, within a body is an important aim. The most suitable procedure is to measure the temperature in situ, but it is not possible by the design of structure. There are some analytical solutions of the very simple unsteady temperature distribution, but they fail when the shape of the structure is complicated. We present a finite element method of the temperature distribution as well as the analysis of the stress within the 3D domain using the same tetrahedron element. Using the theory mentioned above we compiled a set of the procedures for a non-linear analysis of the composite structures with a change of matrix of moduli of elasticity. Some results of the analysis reached by these procedures are presented.

DUALITY BASED DOMAIN DECOMPOSITION WITH ADAPTIVE NATURAL COARSE GRID FOR CONTACT PROBLEMS

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In our paper, we consider frictionless coercive and semicoercive contact problems of elasticity, so that our analysis includes bodies that admit some rigid body motion. Starting from a discretized variational inequality that describes the equilibrium of bodies in contact, we first reduce the problem by duality to a strictly convex quadratic programming problem with simple bounds and possibly with some general equality constraints. This step is closely related to the FETI domain decomposition method of the Neumann-Neumann type proposed by Farhat and Roux for the solution of linear problems. Then a variant of the augmented Lagrangian method is used to solve the resulting problems. The method generates approximations for the Lagrange multipliers for equality constraints in the outer loop while auxiliary quadratic programming problems with simple bounds are solved in the inner loop. The algorithm in the inner loop uses projections and adaptive precision control for the solution of auxiliary problems, so that it can efficiently identify the contact interface. The precision of the solution of the auxiliary problems in the outer loop is controlled by the norm of the violation of the equality constraints.

Then we show how to adapt the natural coarse grid projectors proposed by Farhat and Roux to preconditioning of auxiliary problems in the inner loop of the algorithm. In particular, it turns out that these projectors at the same time decompose the Hessian of the augmented Lagrangian, so that its effective spectral condition number depends neither on the penalization parameter nor on the rank of the penalization term. The procedure can be made even more efficient if we use projectors to the intersection of the current face with the natural coarse grid. Further improvement of the algorithm is achieved by application of the standard preconditioners and auxiliary decomposition.

Finally, we review basic theoretical results that concern the algorithm. It is shown that the algorithm converges to the solution and that the rate of convergence to the solution of auxiliary linear problems is optimal in the sense that the number of iterations depends on the ratio of the decomposition and the grid parameters in spite of the penalization term in the augmented Lagrangian. An error estimate for approximations of the Lagrange multipliers is given that does not have any term that accounts for inexact solution of the auxiliary problems. The performance of the algorithm has been tested on the solution of a 3D elasticity problem and a model variational inequalities decomposed to hundreds subregions. Even the results achieved in serial implementation indicate that there are realistic problems which can be solved very efficiently by the algorithm presented. We believe that the algorithm presented extends naturally the scope of applications of both the original FETI method and its recent improvements to problems described by variational inequalities.

VARIABLE STEP SIZE ROSENROCK SCHEMES FOR THE ADAPTIVE SOLUTION OF NONLINEAR PARABOLIC SYSTEMS

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Diverse physical phenomena are modelled by systems of nonlinear parabolic differential equations (PDEs). Nowadays there is an increasing activity in mathematics to analyse the properties of such models. Due to the great complexity only little is known about true solutions. That is why the numerical analysis of PDEs is the central tool to assess the modelling process for large scale physical problems. In fact, a posteriori error estimates can be used to judge the quality of a numerical approximation and to determine an adaptive strategy to improve the accuracy where needed. In such a way numerical and modelling errors can be clearly distinguished with the effect that the reliability of the modelling process can be assessed. Moreover, successful adaptive methods lead to substantial savings in computational work.

We present an adaptive algorithm to compute solutions of nonlinear PDEs

$$H(x, t, u) u_t = \nabla \cdot (D(x, t, u) \nabla u) + F(x, t, u, \nabla u), \\ x \in \Omega \subset R^n, n = 1, 2, 3, t > 0$$

with additional boundary and initial conditions.

We first discretize in time using linearly implicit one-step methods of

Rosenbrock type possibly of high order with automatic step size control. Starting with the solution u_k at the time t_k , the solution u_{k+1} at the advanced time $t_{k+1} = t_k + \tau_k$ is computed by the following

linear combination of u_k and different intermediate stage values l_j

$$u_{k+1} = u_k + \sum_{j=1}^s b_j l_j$$

with suitable chosen real values for the coefficients b_j . It is the main structural advantage of Rosenbrock-type methods that each of these functions l_j is the solution of a linear elliptic problem.

There is no problem to construct schemes with optimal linear stability properties for stiff equations. By embedding techniques we get an estimation of the temporal discretization error which is used to control the time step.

The elliptic subproblems for the l_j are discretized by an adaptive multilevel finite element method. A posteriori estimates of the spatial error are obtained by solving local Dirichlet problems with higher accuracy.

This strategy of mesh controlling in time and in space is implemented in the code KARDOS and proved to be efficient in a large range of applications.

In an example from 3D-hyperthermia treatment we present computations of the nonlinear heat-transfer in the complex geometry of a human body. Additionally, we show some results about the phenomena of biochemical spot replication and pattern formation.

ADAPTIVE FINITE VOLUME – FINITE ELEMENT SCHEMES FOR COMPRESSIBLE NAVIER-STOKES EQUATIONS

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This paper is concerned with numerical simulation of viscous high speed gas flow modelled with the aid of compressible Navier-Stokes equations. In the solution of this problem several important obstacles must be overcome: convection dominating over diffusion, shock waves, boundary layers, their interaction and, on the other hand, the lack of theoretical analysis of the continuous problem. We have developed a robust theoretically based numerical method for the solution of viscous compressible flow applicable on unstructured meshes.

The viscous terms in the system of governing equations consisting of the continuity equation, Navier-Stokes equations and energy equation are considered as a perturbation of the inviscid Euler equations. Therefore, the method is based on a general class of flux vector splitting cell centred finite volume schemes. The viscous terms are discretized by the finite element method over a triangular grid. Several combined inviscid - viscous finite volume - finite element approaches using suitable mutually consistent finite volume - finite element meshes were developed. Namely, the original triangulation is used for the conforming finite element approximation, while the finite volume method is applied on the dual mesh. Quite another finite volume - finite element approach is proposed for triangular finite volumes. In this case an adjoint finite element triangular grid is constructed to the original finite volume triangulation. Barycentric finite volumes are associated with nonconforming finite element approximation of viscous terms.

Special attention is paid to adaptive mesh refinement techniques playing an important role in the precise resolution of shock waves, boundary layers, wakes and other details of the flow field. We shall discuss several adaptive mesh refinement strategies which we have developed: a) method using a shock indicator with divided density differences taking into account the flow direction, and allowing the correct identification of zones with shock waves, b) method based on the residual error indicator, c) special method leading to anisotropic mesh refinement. Particularly the last approach is very efficient. It leads automatically to the grid alignment along shock waves, identifies boundary layers and other features and optimizes the number of elements necessary for precise resolution of the flow.

A number of technically relevant computations compared with experimental data will be presented, showing the applicability and robustness of the developed methods.

EFFECTIVE SOLUTION OF LARGE SYMMETRIC EIGENVALUE PROBLEMS BY COMBINED MULTI-GRID AND RAYLEIGH QUOTIENT METHODS

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This paper presents computational procedures related to employing Multi-Grid (MG) techniques in the context of the modified Rayleigh Quotient (RQ) method for the solution of a few smallest eigenpairs of very large symmetric systems arising in finite element simulation of 3D structural dynamic problems.

The standard RQ method is modified by replacing the correction equation with mathematically equivalent alternative equations which are more well-defined to be solved by iterative solvers such as MG approaches. The Jacobi-Davidson equation and the so-called inflated Newton recurrence have been chosen as two alternative equations for further investigation.

The MG approach concerned plays two roles in this combined solution strategy: Firstly, at each grid, a local solution is sought first and then adopted as an initial guess for the next finer grid. This can be achieved by recursively applying the current solution method to the next coarser grid until the coarsest grid is reached or at some grid where the solution can be effectively found by using conventional techniques such as the Lanczos method. Secondly, the MG approach is employed to solve the correction equation in the inner loops of the RQ method. The MG solver considered here has the following features: (1) the grids can be totally non-nested and unstructured; (2) the coarse grid equation can be derived independently or in a Galerkin manner; (3) any (preconditioned) iterative solver can be employed as pre- and post-smoothers; (4) each MG iteration cycle is further accelerated and stabilized by the (Flexible) GMRES algorithm, which is equivalent to a MG preconditioned (F)GMRES method.

As the correction equation is solved only approximately, the convergence properties of the original RQ method are no longer valid. In this situation, a local 2 X 2 Ritz-Galerkin analysis is performed at each RQ iteration, which turns out to be vital for achieving a high performance.

Finally, a set of very large eigenvalue problems (over 100,000 DOF) is presented to illustrate the performance of the proposed solution. In addition, the effects of some parameters associated with the method on the overall performance are also investigated.

THE METHOD OF TRANSPORT FOR CONVECTION-DIFFUSION EQUATIONS

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The Method of Transport was introduced by M. Fey as a genuinely multi-dimensional finite volume scheme to solve the compressible Euler equations. In Euler equations physical information travels in all direction. The basic idea is to decompose this moving information in finitely many parts, each being advected in another direction. Each 'wave' is modeled by a linear advection equation, where the coefficient depends on the space variable only.

For the simulation of compressible viscous flows one uses the Navier-Stokes equations. Here the diffusion process does act in all directions, similar to the acoustic waves in the Euler equations. We take this into account by choosing finitely many waves. Hence one decomposes the system into linear advection equations. The resulting scheme is first order. Introducing corrections terms one obtains a second order scheme. These terms look like a viscosity but with a negative sign, because they damp the numerical viscosity. To derive the scheme we first study the advection-diffusion equation.

MULTISCALE MODELS FOR PROBLEMS IN HETEROGENEOUS MEDIA

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In analyzing composite structures it is common in practice to carry out distinct levels of analysis corresponding to different length scales: (i) macroscale (structural level), (ii) mesoscale (laminate level), and (iii) microscale (the level of microconstituents). On the structural level structural components are treated discretely, while individual plies are not recognized, except in determining the stiffness of the shell. On the laminate level, individual plies are treated discretely, while microconstituents are treated collectively as a homogenized medium. These steps comprise a sequence of interdependent analyses in the sense that the output from one level is used as input to the next level, where constitutive laws serve as bridging mechanisms between the scales. In this talk we show that for certain class of problems, such as in the case of woven or textile composites, the coupling between the scales is so profound that a series of uncoupled analyses may lead to poor predictions of local and global fields. This is in particular true in the areas of high gradients, primarily developed at the boundary layers. A typical unit cell size for a woven microstructure ranges from 3mm for plane weaves to more than 10mm for 3D woven composites. Thus the unit cell size for textile or woven composites could be of the same order of magnitude as the small geometrical feature, such holes and cutouts, in the macrostructure.

FAR-FIELD BOUNDARY CONDITIONS FOR FINITE ELEMENT APPROXIMATION OF VASCULAR FLOW PROBLEMS

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In the numerical modelling of blood flow in cardiovascular districts, the boundary treatment of domains which have been artificially truncated for computational purposes is a major numerical issue. Two aspects are of relevance.

The first is linked to the fact that if a 2D or 3D model is employed there is a lack of boundary data available for the Navier Stokes equations that are adopted to describe the flow. Suitable pointwise boundary conditions are seldom available in practice and most often only integrated quantities on selected sections are provided, such as mean pressure or mean flow-rate. One of the scope of our analysis is to investigate a correct mathematical setting for these defective boundary conditions, and to assess at which extent they are computationally effective.

The second aspect is the necessity of taking into account a feed-back mechanism: the vascular district under numerical study is part of a more complex system with which it interacts. An advanced approach we are investigating is based on coupling the Navier-Stokes equations with a lumped parameter models of the whole cardiovascular system. An iterative mechanism that activates both the detailed and the lumped parameter models through appropriate flux exchange at the interface will be proposed. This hybrid approach is potentially very interesting as it can combine the low computational complexity of a lumped parameter model with the local accuracy of a distributed one.

A last point that will be analysed concerns the appropriate non-reflecting conditions for the fluid-structure interaction problem arising when the deformability of the vessel wall is taken into account. As a matter of fact, the numerical control of the spurious pressure waves that are originated by the compliant vessel is of outmost importance for the overall reliability of the numerical model.

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AN ENHANCED ERROR ESTIMATOR ON THE CONSTITUTIVE RELATION FOR NONLINEAR TIME DEPENDENT PROBLEMS

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One important research topic is the mastery of F.E. computations in nonlinear time-dependent analysis. For such computations, the quality of the finite element solution at t depends not only on the quality of the mesh, but also on the quality of the time discretization used since the beginning of the loading. Mastering such an analysis is thus clearly more complex than in the case of linear static problems. In particular, an approach which consists of directly applying the procedures used in statics, at certain time steps, is insufficient in estimating the quality of such a computation. It is therefore necessary to build error measures that allow, over the whole time interval $[0, T]$, taking into account all of discretizations errors. Errors possessing these properties have been developed from an a posteriori error estimator based on the error on the constitutive relation [1].

We present an extension to non-linear problems of a new error estimator on the constitutive relation proposed by P. Ladevèze [2] for linear elastic problems. we will consider herein the Drucker-type error estimator [3]. Drucker's error estimator uses the same technique for contructing the equilibrated stress fields as in linear analysis; this technique is independent of the constitutive relation. However, the quality of our error estimator depends on the quality of the equilibrated stress field recovery. In order to improve the quality of our estimate, a new construction technique, derived from [2] and which takes into account both the constitutive relation and the error measure, is presented. Numerical experiments show that this enhanced error estimator can lead to a significant improvement in the effectivity indexes in the case of anisotropic meshes, or when quasi-perfect plasticity is approached.

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BOUNDARY ELEMENT METHODS FOR SOME NONLINEAR PROBLEMS

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In this work, we are interested in computing an isolated harmonic solution u of the nonlinear boundary value problem described by

$$\Delta u(x) = 0 \quad \text{for } x \in \Omega \subset \mathbb{R}^n \quad (n = 2, 3) \quad (1)$$

and the nonlinear boundary condition

$$\frac{\partial}{\partial n_x} u(x) + g(x, u(x)) = f(x) \quad \text{for } x \in \Gamma, \quad (2)$$

where Ω is a bounded domain with a Lipschitz boundary Γ . In (2), n_x is the outer normal unit vector defined almost everywhere for $x \in \Gamma$ and $f : \Gamma \rightarrow \mathbb{R}$, $g : \Gamma \times \mathbb{R} \rightarrow \mathbb{R}$ are given functions.

Application of the above model include the steady-state diffusion equations. We impose some appropriate mild conditions on the nonlinearity involved. Boundary integral formulations are useful to compute solutions of (1) and (2). We derive some novel nonlinear boundary integral equations which are equivalent to (1) and (2) and have excellent computational advantages.

The first formulation is obtained through the Dirichlet–Neumann map and the second one follows from an indirect double layer potential ansatz. The indirect hypersingular formulation is computationally more efficient than the Steklov–Poincaré operator formulation, but the solution has some regularity restrictions compared with the solution of the equation involving the Steklov–Poincaré operator. Hence, we will propose later a hybrid solution strategy based on both formulations.

Our first step in solving the nonlinear boundary integral equations is to use a Newton scheme to approximate the continuous nonlinear problems by a sequence of perturbed linear first kind boundary integral equations involving either the Steklov–Poincaré operator or the hypersingular integral operator. We show that each of these continuous linear problems are stable and the solutions converge to an isolated solution of the associated nonlinear boundary integral equation.

To solve the sequence of Newton iterate linear boundary integral equations we use some practical variants of the Galerkin boundary element method which retain the self-adjointness and positivity properties in the discrete problems.

The implementation of the Galerkin schemes for Newton iterate continuous linear problems result in solving a sequence of dense matrix equations. At each step, these are to be solved efficiently using suitable fast iterative techniques in combination with efficient preconditioners. To our knowledge, our present work is the first in initiating

and analysing preconditioners for a sequence of linear systems arising from boundary element methods applied to a new class of nonlinear boundary integral equations. We use a preconditioning technique based on an integral operator of opposite order which requires minimal standard assumptions on the mesh, typically suited to linear problems on non-smooth boundaries.

COMBINATION OF MIXED-FEM AND DTN MAPPINGS FOR NONLINEAR EXTERIOR TRANSMISSION PROBLEMS

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We combine primal and dual mixed finite element methods with suitable Dirichlet-to-Neumann mappings to study the solvability and Galerkin approximations of nonlinear exterior transmission problems arising in plane elasticity and potential theory. As model problems, we consider a nonlinear incompressible material and a nonlinear elliptic equation in divergence form, coupled with an incompressible elastic material and the Laplace equation, respectively, in an unbounded region of the plane. The corresponding Dirichlet-to-Neumann mapping is derived by using Fourier series expansions, for the first case, and the boundary integral equation method, for the second one. We establish existence and uniqueness of solution for the continuous and discrete variational formulations, and provide the corresponding error analysis for appropriate finite element subspaces. The main tool of our analysis is given by a generalization of the usual Babuška-Brezzi theory to nonlinear variational problems with constraints.

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ON APPLICATIONS OF BOUNDING ENERGY THEOREMS IN COMPUTATIONS OF DEFORMABLE SYSTEMS

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Several inequalities concerning the elastic energy in discretised deformable systems were derived by the author in 1993 (Arch. Mech., 45, 4, 439-455). The problem was considered in the frame of kinematically linear theory using FEM-oriented description (due to G. MAIER, e.g. Comp. & Struct., 7, 1977, 599-612). The distortional approach has been used in this paper. So, all deformations due to physically non-linear properties have been treated as effects of the presence of distortions imposed on the linear elastic structure. The inequalities are obtained from the positive definiteness of the elasticity matrix, from the equilibrium equations and from the kinematic compatibility conditions only, and therefore the range of their validity is rather very wide. The specific form of the inequalities allowed the author to formulate bounding energy theorems (including also the complementary energy) to linear elastic, elastic-plastic and slackened-elastic-plastic structures with arbitrarily distributed additional strain distortions. The bounding theorems cover a wider class of problems than the variational principles. In general, they determine the upper or lower bounds on the functional or function under consideration. However, the true solution may not correspond in general to the lower or upper bound, specified in the bounding theorems. Obviously, all extremum principles are also bounding theorems but, in that case, the true solution corresponds to the stationary point of the functional.

The fundamental inequalities can be numerically applied to insufficiently recognised problems, where some intuitively acceptable assumptions are introduced. In such cases the energy bounds can be used in order to check the correctness of computer calculations.

The formulation of bounding theorems for a continuum will be presented at the conference. Some applications of the energy bounds to the estimation of elastic energy variations in simple slackened-elastic-plastic systems will be presented. The calculation show that the elastic energy in such systems may be non-monotone function of monotone increasing loadings. However, it should be noted that the description used in the work allows us to consider much more complex systems, including also 3D structures. The results of the work can be also applied in damage mechanics, where the elastic energy plays a very important role. It should be added that the fundamental inequalities include in special cases the well-known results in the literature of the subject (e.g. Hodge's theorem, the elastic energy in elastic-cracking bodies).

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FAST INFINITE ELEMENT METHODS

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Infinite Element Methods (IEM) are computationally efficient methods to solve exterior acoustic problems and are more than an alternative to the standard Boundary Element Methods (BEM). The computational efficiency of the IEM results from the fact that a 3D problem is solved by only using a 2D numerical quadrature, because the third directions is integrated analytically ahead of time. This type of integration over the 3D domain leads to the computational efficiency of the methods although a linear system stemming from the discretization of the 3D domain has to be solved. Recently, the standard BEM has been extended and the use of wavelet basis functions has eliminated the disadvantages of the standard BEM, namely a dense stiffness matrix and the prohibitive computational cost. This obviously shows that it is necessary to further develop and increase the efficiency of the IEM. One possible approach that is treated in this work is to borrow spectral element techniques and to apply them to the finite element part, the 2D integration, in the IEM. In detail, we do not choose the 2D finite element shape functions independent of the integration rule. Instead we combine them and accept a slight loss in accuracy of the quadrature rule. This significantly enhances the computational efficiency of the numerical scheme. The numerical results clearly show the speed up that can be achieved by applying such techniques.

MULTILEVEL EVALUATION OF BOUNDARY INTEGRAL OPERATORS

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The evaluation of discretized boundary integral operators is the most time consuming part for the numerical solution of boundary integral equations. We present a multilevel evaluation algorithm for the fast application of integral operators which is based on the ideas of Brandt and Venner. We extend this method from one-dimensional integral transformations to boundary integral operators on complicated two-dimensional manifolds in the three-dimensional space. Furthermore, we combine the multilevel evaluation with the Galerkin-boundary element method to obtain a robust discretization scheme. Then we analyze the algorithm with respect to costs and accuracy and finally, we present some numerical results.

A SURVEY ON COMPRESSION METHODS FOR BOUNDARY ELEMENT MATRICES

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The last 15 years have seen a tremendous advance in the numerical treatment of boundary integral equations through the boundary element method. One of the most difficult parts of it is the efficient evaluation of the

discretized integral operator. Several approaches have been made to overcome this problem, e.g., panel clustering, fast multipole method, wavelet-compression, skeleton approximation and multilevel evaluation. The aim of the talk is to present all these methods inside one general framework. This will elucidate their common ground as well as their differences.

A HIERARCHY OF OPTIMAL NON-REFLECTING FINITE ELEMENTS

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A class of numerical methods to solve problems in unbounded domains is based on truncating the infinite domain via an artificial boundary \mathcal{B} and applying some boundary condition on \mathcal{B} , which is called a Non-Reflecting Boundary Condition (NRBC). Here, a systematic way to derive *optimal local NRBCs* of given order is developed in various configurations. The optimality is in the sense that the local NRBC best approximates the exact nonlocal Dirichlet-to-Neumann (DtN) boundary condition for C^∞ functions in the L_2 norm. The optimal NRBC may be of low order but still represent high-order modes in the solution. The optimal NRBCs are combined with finite element discretization in the computational domain.

The optimal NRBCs are applied to various unbounded domain problems. These include the Laplace and Helmholtz equations in exterior and wave-guide configurations, as well as the time-dependent scalar wave equation, which is treated in a semi-discrete manner.

The theoretical properties of the resulting class of schemes are examined. In particular, theorems are proved regarding the numerical stability of the schemes and their rates of convergence. In addition, the performance of the optimal NRBCs in conjunction with a standard finite element scheme is demonstrated via numerical examples.

NUMERICAL APPROXIMATION OF EIGENVALUE PROBLEMS IN INTEGRATED OPTICS

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This work is devoted to the numerical computation of the guided modes of the dielectric stratified waveguides.

A waveguide in integrated optics can be seen as a cylindrical domain of propagation which allows the electromagnetic energy to be confined inside, at least for certain frequencies depending on the geometry of the medium and on the refraction index of the materials of which it is composed.

We consider an open stratified waveguide translationally invariant in the infinite propagation direction x_3 . Its cross-section is also supposed to be an unbounded and stratified medium where an appropriate perturbation of the refraction index $n(x_1, x_2)$ has been introduced to ensure the existence of guided modes.

Mathematically, the problem to be solved can be reduced, under the hypothesis of weak guidance, to

$$(\mathcal{P}) \quad \left\{ \begin{array}{l} \text{Find } \omega > 0 \text{ and } u \neq 0, \quad u \in H^2(R^2) \quad \text{such that} \\ -\Delta u + \beta^2 u = \omega^2 n^2 u \end{array} \right.$$

For a given $\beta > 0$, called the *propagation constant* of the mode, (\mathcal{P}) is a scalar selfadjoint eigenvalue problem set in the cross section of the waveguide where the square of the *frequency*, ω^2 , plays the role of eigenvalue.

The main difficulties to solve this problem come from the unboundedness of the cross section and the stratified nature of the medium.

The method we propose for the computation of the guided modes appears as a combination of analytical methods, which take into account the unboundedness of the propagation medium, and numerical computations which can be reduced to a neighborhood of the perturbation.

Problem (\mathcal{P}) is shown to be equivalent to find, for $\beta > 0$ given, the values of $\omega > 0$ which makes 0 to be an eigenvalue of an elliptic operator $S(\omega, \beta)$. This operator is numerically computed via a decomposition in the form

$$S(\omega, \beta) = S_i(\omega, \beta) - S_e(\omega, \beta) + S_p(\omega, \beta)$$

where S_i , S_e and S_p correspond to solution operators of three boundary value problems: Two of them are set up in the homogeneous parts of the layered medium while the third one treats the inhomogeneous, but local, perturbation.

Some numerical results obtained for different test cases are presented.

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IMPLEMENTATION OF FAST INTEGRATION METHODS IN 3D BOUNDARY ELEMENTS

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In this talk we describe the implementation of the fast integration techniques for boundary elements introduced in recent joint papers by I.G. Graham, W. Hackbusch and S.A. Sauter.

In these techniques most of the stiffness matrix arising in a boundary element method is computed by node-based quadrature rules, the weights of which have to be computed in a first phase of the matrix assembly process. This constitutes an $O(N)$ process, which in practice is a small fraction of the overall assembly time.

Once these weights are computed the matrix is assembled by an adaptive routine which uses the node-based quadrature rules wherever possible and only conventional element-based rules for a small number of singular or nearly singular elements.

We describe the general principles behind the implementation of this algorithm and illustrate these with computational experiments involving boundary integral equations on a selection of smooth and non-smooth surfaces. The experiments show that theoretical predictions are realisable in practice for a variety of problems, even including the strongly anisotropically refined meshes commonly used for approximation of edge singularities.

BODY-BODY CONTACT SOLVERS BASED ON NEUMANN DD TECHNIQUES

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This talk deals with the construction of efficient algorithms for the solution of the finite dimensional constrained minimization problem arising from the finite element discretization of contact problems.

Dualization techniques have been used to decrease the problem size from the large number of unknowns in the domain to the much smaller number of inequalities at the boundary. The disadvantage of this direct Schur-complement approach is the full matrix of the dual problem.

Domain decomposition techniques meet very similar requirements. A global boundary value problem is decoupled into local subproblems, and one interface problem at the (coupling) boundary. Two complementary approaches are the Dirichlet method and the Neumann method. The first one requires preconditioners for local Dirichlet problems and for the interface problem in $H^{+1/2}$, and extension operators from the boundary into the domain. The later one needs preconditioners for local Neumann problems, and for the interface problem in $H^{-1/2}$.

Efficient multi-level algorithms for all components are available in literature.

In this talk it is shown how to use exactly these components for the construction of solvers for contact problems. For body body contact problems the Neumann version seems to be easier to implement.

We will present a stabilization technique based on the complementary condition. It has positive effects on the accuracy of the discretization as well as on the mapping properties of the arising operators.

Numerical results for 2d and 3d will be presented. The examples verify the theoretical results concerning optimal convergence of the algorithms. We present experiments with a posteriori error estimators combining residual terms and penetration terms.

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TREFFTZ INFINITE ELEMENTS FOR ACOUSTICS

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Trefftz infinite elements for exterior problems of time-harmonic acoustics are presented. The formulation is based on a functional which provides a general framework for domain-based computation of exterior problems. The exterior problem is partitioned into an inner field in a bounded domain and an outer field in its unbounded complement. Normal derivatives weakly enforce continuity across the interface. For smooth representations of the outer field there is no integration over the unbounded domain.

Infinite elements are usually based on piecewise smooth functions. In this case we account for possible discontinuities across infinite element boundaries by incorporating a jump term in the formulation. Two prominent features simplify the task of discretization: the infinite elements mesh the interface only and need not match the finite elements on the interface.

Various infinite element approximations for two-dimensional configurations with circular interfaces are reviewed. Numerical results demonstrate the good performance of these schemes. A simple study points to the proper interpretation of spectral results for the formulation. The spectral properties of these infinite elements are examined with a view to the correct representation of physics and efficient numerical solution.

For three-dimensional configurations with spherical interfaces the infinite element interpolation is based on separation of variables in a spherical system. The lowest-order element approximations combine piecewise-linear azimuthal interpolation, latitude variation described by associated Legendre functions, and oscillatory outgoing radial behavior. Singularities at the poles require careful consideration.

NODAL FINITE ELEMENTS FOR MAXWELL'S EQUATIONS: HOW TO DEAL WITH GEOMETRIC SINGULARITIES

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In this communication we are concerned with the time-harmonic Maxwell equations which are given in a **regularized form** similar to the vector Helmholtz equation. In the case of a regular or convex domain, this problem can be discretized by means of nodal finite elements. Here, we are interested in the same problem in a **non-convex polyhedron**. The mathematical analysis dwells on two rather different situations, depending whether we consider a **perfect conductor** or an **impedance boundary condition**.

In the first case we show that a nodal Finite Element Method does not approach in general the solution to Maxwell's equations, since the electromagnetic field presents **singularities** near reentrant edges and corners of the domain which cannot be approximated by Lagrange finite elements. From a mathematical point of view, this is due to the boundary condition of a perfect conductor. Indeed, the formal approach leads to **two variational formulations** involving the same sesquilinear form, but different functional spaces. For a regular domain, these spaces coincide, whereas in the case of a non-convex polyhedron, one is a **closed sub-space** of the other and does not contain the singular fields. Hence, the solutions to the corresponding variational problems do not coincide in general, and only one of them has a physical interpretation. In particular, we show that a nodal Finite Element Method necessarily converges to the "wrong" solution, i.e. the one which does not represent the electromagnetic field. Therefore, mesh refining (which is often used in the case of poor convergence rates, for example, in elasticity problems) will fail!

To come accross the difficulty of the regularity gap, we propose a new method involving the **decomposition of the electromagnetic field** into a regular part that can be treated numerically by nodal finite elements, and a singular part that is determined and taken into account explicitly. This **singular field method** applies to various situations and numerical results will illustrate the approach in the 2D case.

In the case of an **impedance boundary condition**, the situation is rather different. Indeed, we are able to prove a **density result** of regular fields for the functional space involved in the variational formulation. This allows a discretization by means of **nodal finite elements**, contrary to the case of a perfect conductor.

A DOMAIN SPLITTING METHOD FOR HEAT CONDUCTION PROBLEMS IN COMPOSITE MATERIALS

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The present investigation has been carried out in cooperation with K.-H. Hoffmann (Bonn) and Yu. A. Kuznetsov (Houston). — We consider a domain decomposition method for some unsteady heat conduction problem in composite structures. This linearized model problem is obtained by homogenization of thin layers of fibres embedded into some standard material. The set of finite element equations obtained by the backward Euler scheme is parallelized in a problem-oriented fashion by some noniterative overlapping domain splitting method, eventually enhanced by inexpensive local iterations to reduce the overlap. We present a detailed convergence analysis of this algorithm which is particularly well appropriate to handle fibre layers of nonlinear material. Special emphasis is to take into account the specific regularity properties of the present mathematical model. Numerical experiments show the reliability of the theoretical predictions.

**THE FOURIER-FINITE-ELEMENT METHOD FOR TREATING
EDGE SINGULARITIES OF SOME ELLIPTIC PROBLEMS
IN AXISYMMETRIC DOMAINS**

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The Fourier-finite-element method, which combines the approximating Fourier and the finite-element method, is applied to Poisson-like equations with interfaces and to the Lamé equations in three-dimensional axisymmetric domains $\hat{\Omega}$. Edges on the interfaces or on the boundary that lead to singularities of the solution $\mathbf{u}(r, \varphi, z)$ (r, φ, z : cylindrical coordinates) are admitted. The partial Fourier decomposition with respect to the rotational angle φ reduces the three-dimensional boundary value problem to a sequence of decoupled two-dimensional boundary value problems on the meridian plane Ω_a of $\hat{\Omega}$. Their solutions $\mathbf{u}_n(r, z)$ ($n = 0, 1, \dots$) are the Fourier coefficients of the solution $\mathbf{u}(r, \varphi, z)$; they can be calculated independently from each other. Appropriate function spaces on the meridian domain Ω_a are given to characterize the two-dimensional problems. Moreover, completeness relations coupling the two- and three-dimensional problems as well as trace properties (on the rotational axis) and a priori estimates of the Fourier coefficients \mathbf{u}_n are proved. Tensor and non-tensor product representations of the edge singularity functions are taken into account. They are studied by Fourier series expansion and numerically treated by appropriate local mesh grading in the meridian plane Ω_a around the corner generating the edge. Moreover, the approximate calculation of stress intensity coefficients is also considered. By using some mixed projections and estimation techniques it can be proved that the degree N of the trigonometric polynomials and the mesh size h of the triangular mesh (with piecewise linear elements) occurring in the error estimates are not coupled (anisotropic discretization) and that the energy norm of the error of the Fourier-finite-element approximation behaves like $O(h + 1/N)$, i.e., it is of the same order as for regular solutions. The talk also includes recent results of joint work with S. Nicaise and B. Nkemzi.

CONTAMINATION OF SOILS AND GROUNDWATER FROM VOLATILE ORGANIC COMPOUNDS

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Contamination of soils and groundwater from volatile organic compounds (VOC's), such as organic solvents and hydrocarbon fuels, is a problem at many industrial facilities. Key to the characterization of surface contamination conditions, and to the design and implementation of ineffective remediation strategies, is an understanding of the physical, chemical, and biological processes on different scales that affect the behavior of contaminants in the subsurface environment. Based on the character of the available data, we need a corresponding model concept which correctly represents the physical processes. The first part of the talk will discuss how scale and system dependent processes and parameters are incorporated into a conceptual model. Next, a robust and effective numerical algorithm for representing the aforementioned concepts will be presented. In addition, two examples involving a three-phase, three-component model for the remediation process of heat injection and the scale dependence of model parameters will be provided.

DOMAIN DECOMPOSITION FOR HIGH ORDER BOUNDARY ELEMENT METHODS

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We present preconditioners for the p and $h-p$ versions of the Galerkin boundary element method for first kind integral operators on surfaces Γ . The arising linear systems are fully occupied and ill-conditioned. Our preconditioners are based on specific decompositions of the ansatz spaces. For operators of order one continuous ansatz functions are required. Here, the analysis is carried out within $H^{1/2}(\Gamma)$ which is the trace space of H^1 on a three-dimensional domain with trace Γ . On the other hand, the energy space of operators of order minus one is the dual space of $H^{1/2}(\Gamma)$ and, here, continuity of the trial functions is not needed.

In order to define our preconditioners we introduce a coarse grid with elements of size H_j . These elements are the subdomains which define the basic decomposition of the ansatz spaces of piecewise polynomials of high degrees on finer meshes. We require that the fine meshes are locally quasi-uniform, i.e. they are quasi-uniform on subdomains. Within $H^{1/2}(\Gamma)$ the coarse mesh decomposition is part of a three-level method where the first two levels deal with piecewise polynomials of degree one. For operators of order minus one the decomposition given by the coarse mesh is part of a direct sum decomposition of the full ansatz space. Here, only piecewise constant functions on the coarse mesh are taken as a global subspace.

In both cases the condition number of the preconditioned linear systems is bounded

by $\max_j(1 + \log(H_j p_j / h_j))^2$. Here h_j is the mesh size of the fine mesh in the subdomain with size H_j , and p_j is the maximum polynomial degree in that subdomain.

The theoretical bounds on the condition numbers are confirmed by numerical experiments.

EFFICIENT IMPLEMENTATION OF HP FINITE ELEMENT METHODS

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Although the superior convergence properties of hp type finite element approximations are well known and have been studied in detail, implementations of hp methods for practical applications are not yet widespread.

Among the reasons are, the lack of suitable mesh generators producing coarse, locally refined meshes, and a common belief that higher-order finite element methods are slow and hard to implement.

In our contribution, we analyze all steps of *hp* finite element analysis - from automatical mesh generation to stiffness matrix setup, equation solving, and result evaluation - and present strategies for handling these tasks efficiently. Problems covered are Reissner Mindlin plate bending and plane elasticity, with remarks extending to higher-order plate models and to elasto-plasticity.

We address the problem of suitable data structures for storing hp finite element discretizations. One of the main points is that hp finite element methods require a more detailed description of the topological adjacency relations than traditional *h*-version codes. We need edge-based adjacency information in order to ensure the continuity of the approximation, as well for evaluating residual-based error indicators. In order to introduce mesh refinements for capturing local effects like boundary layers or point singularities, we also need comprehensive topological information.

Next, we address the problem of loadcase superposition. In our view, each loading or boundary condition case requires a specifically tailored finite element approximation, so that extremum finding and loadcase superposition for various loadcases cannot be carried out on the basis of a fixed finite element mesh. Instead, an additional mesh, called auxiliary mesh, is required.

The next topic is coarse mesh generation. We present an approach based on a mesh density distribution computed as the solution of an auxiliary Laplace problem, utilizing once more the auxiliary mesh. Also, we show techniques for creating refined meshes with point refinements and boundary layer refinements.

Next, we consider the integration of the element stiffness matrices. This seems like a very time-consuming task for high *p* levels, but this impression is not really true, as will be demonstrated next.

Then, we discuss the problem of assembling and storing a matrix of p-elements efficiently. We present two approaches, both of which require only $O(N \log(N))$ operations, where N is the total number of unknowns.

We give some remarks on numerical experiences with various equation solving strategies.

Finally, we discuss strategies for fast result evaluation.

We conclude with an extension to elasto-plastic computations, and we discuss the role of the auxiliary mesh in this context as well.

Time and equipment permitting, the talk will be accompanied by a live presentation illustrating the main points.

A POSTERIORI ERROR ANALYSIS OF STABILISED FINITE ELEMENT METHODS FOR HYPERBOLIC PROBLEMS

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We develop the *a posteriori* error analysis of stabilised finite element approximations of first-order hyperbolic problems, including the streamline diffusion method and the least-squares stabilised finite element method. In particular, we discuss the question of error estimation for linear functionals, such as the outflow flux and the local average of the solution.

Due to the presence of the stabilisation parameter δ , a conventional duality argument leads to an error bound that is not equilibrated. We propose an alternative approach which exploits a δ -dependent dual problem that respects the Galerkin property of the stabilised method; this enables us to derive an equilibrated *a posteriori* bound on the global error which exhibits the full approximation power of the finite element space. The theoretical results are illustrated by numerical experiments.

This research has been carried out in collaboration with Endre Süli (University of Oxford) and Rolf Rannacher (University of Heidelberg).

HYBRID COUPLED FINITE-BOUNDARY ELEMENT METHODS FOR ELLIPTIC SYSTEMS OF SECOND ORDER

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In this hybrid method, we consider, in addition to traditional finite elements, the Trefftz elements for which the governing equations of equilibrium are required to be satisfied a priori within the subdomain elements. If the Trefftz elements are modelled with boundary potentials supported by the individual element boundaries, this defines the so-called macro-elements. These allow one to handle in particular situations involving singular features such as cracks, inclusions, corners and notches providing a locally high resolution of the desired stress fields, in combination with a traditional global variational FEM analysis. The global stiffness matrix is here sparse as the one in conventional FEM. In addition, with slight modifications, the macro-elements can be incorporated into standard commercial FEM codes. The coupling between the elements is modelled by using a generalized compatibility condition in a weak sense with additional elements on the skeleton. The latter allows us to relax the continuity requirements for the global displacement field. In particular, the mesh points of the macro-elements can be chosen independently of the nodes of the FEM structure. This approach permits the combination of independent meshes and also the exploitation of modern parallel computing facilities. We present here the formulation of the method and its functional analytic setting as well as corresponding discretizations and asymptotic error estimates. For illustration, we include some computational results in two- and three-dimensional elasticity.

A NEW MESH MOVEMENT ALGORITHM FOR FINITE ELEMENT CALCULATIONS II: TIME DEPENDENT PROBLEMS.

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Following on from its predecessor, this talk demonstrates how the mesh movement algorithm derived in part I can be applied to evolution problems. It addresses issues that do not arise in the static case such as inter-grid transfer or are accentuated in the time dependent case such as mesh quality. Numerical examples for parabolic problems in two spatial dimensions are given.

UNIFIED MOLECULAR DYNAMICS AND HOMOGENIZATION FOR BENTONITE BEHAVIOR: SEEPAGE AND MASS TRANSPORTATION

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In high-level radioactive waste management, it is one of the key issues to predict the behavior of bentonite that is the most important component of the Engineering Barrier System (EBS) for containment of radioactive species. However any existing macro-phenomenological models are essentially insufficient for assessing the true seepage and mass transportation behavior of bentonite clay.

Clay is a typical micro-inhomogeneous material. That is, it consists of clay minerals, macro-grains, water, air and others in its microscopic level. There are two essential issues for analyzing the behavior of such micro-inhomogeneous materials: One is how to determine the characteristics of constituent components of the micro-continuum which are directly affected by their molecular movement, and another is how to relate the microscopic characteristics to the macroscopic behavior. For solving the first problem, we apply Molecular Dynamics method (MD) to determine the material properties of each constituent component, then Homogenization Analysis (HA; Sánchez-Palencia 1980, Bakhvalov & Panasenko 1984) is used for estimating the micro to macro behaviors. This is the unified MD/HA procedure, and we applied this unified method to the time-dependent visco-elastic problem (Kawamura et al. 1997) and the seepage problem (Ichikawa et al. 1998) of bentonite.

The important feature of the unified MD/HA method in the seepage analysis is that it is possible to predict the micro-scale and macro-scale velocity fields simultaneously. Then we can formulate the mass transportation problem without any ambiguous factors such as tortuosity, which are involved in the conventional macro-phenomenological theories. In this paper we discuss how to treat the mass transport field of chemical species in bentonite coupled with the groundwater flow field.

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NEW RESULTS ON THE STABILITY OF A COUPLED FINITE-INFINITE ELEMENT APPROXIMATION FOR EXTERIOR HELMHOLTZ PROBLEMS

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Exterior scattering problems from obstacles of arbitrary shape can be solved using a partition of the exterior domain into finite and infinite elements which are coupled along a so-called artificial boundary. The approximation used in the infinite elements is, in general, of spectral type, being derived from the series representation of the exact solution. In an earlier paper, the authors showed a general estimate for the spectral error of the coupled approximation. The key idea of our analysis is to represent the spectral approximation by a Dirichlet-to-Neumann (DtN) condition on the artificial boundary. The theorem can be applied to various approximations in different variational formulations of exterior problems. The essential step in the application of the general theorem to a concrete boundary value problem consists in the proof of an inf-sup condition for the variational formulation that is used for discretization. In the talk, we consider infinite element formulations for exterior Helmholtz problems (linear acoustics). The radial approximation within the acoustic infinite elements has been derived from the well-known representation theorem of Wilcox. Since the finite and infinite elements are coupled within a *variational* formulation, the corresponding DtN map has to be defined *weakly*. This definition has some surprising consequences on the spectral properties of the discrete DtN operators. We review the results of our computational experiments and discuss the conclusions on the discrete stability of the radial approximation. The experiments are carried out using a model problem where the finite-infinite element discretization is coupled along the unit sphere.

**A PARALLEL DOMAIN DECOMPOSITION ITERATION
SCHEME FOR A HETEROGENEOUSLY MODELED FREE
BOUNDARY PROBLEM**

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The free boundary problem investigated to demonstrate the approach is that of fluid flow past a symmetric truncated concave shaped profile between walls. An open wake or cavity is formed behind the profile. This problem is solved using conformal mapping techniques which yields a formulation in a logarithmic hodograph plane. The solution domain in this plane is then decomposed into two non-overlapping domains. Heterogeneous modeling is used to describe the decomposed problem, i.e. a different governing partial differential equation in each domain. In one of these domains a Baiocchi type transformation is used to obtain a fixed domain formulation for the part of the transformed problem containing an unknown boundary. In the other domain the Baiocchi type transformation is extended across the boundary between the two domains yielding a different problem formulation. This assures that the dependent variables and their normal derivatives are continuous along this common boundary.

A successive over-relaxation finite element collocation approach is applied over the whole problem domain with the use of a projection-operation over only the fixed domain formulated part (the part containing the unknown boundary). The scheme starts by assuming Dirichlet data on the boundary between the two domains for both domains in the first iteration. Neumann data is then obtained from each domain on this boundary, averaged and used as the boundary data for each domain for the next iteration. New Dirichlet data is obtained, averaged and used as the boundary data for the next iteration. The iterations in each domain are done in parallel and continued until the preset error criteria are satisfied. Numerical results are given for the case of a truncated circular profile. These results are compared with other published results and are found to be in good agreement.

FINITE ELEMENT MODELLING OF HELICALLY SYMMETRIC STRUCTURES

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Helically symmetric structures such as helical springs, machine screws and wire rope strands, are commonly used structural items. When they are subjected to axial loads (tensile and torsional), these structures may still exhibit the helically symmetric characteristic after loading. This feature can be used to substantially simplify the analysis of these structures in numerical simulations. The formulation of helically symmetric boundary conditions for finite element modelling is presented. The helically symmetric relationship is ensured by using constraint equations which relate the displacements of the corresponding nodes on the corresponding artificial boundaries of the finite element model. The application of these helically symmetric equations renders it possible to reduce the finite element model size greatly and improve the accuracy of the results. Numerical examples are presented which demonstrate the validity of the formulation.

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**ON OPTIMAL NODE LOCATION IN THE
FINITE ELEMENT SOLUTION OF ELLIPTIC PDES
USING UNSTRUCTURED MESHES IN 2-D**

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Recent work by the author, [P. K. Jimack, Local Minimization of Errors and Residuals Using the Moving Finite Element Method, School of Computer Studies Research Report 98.17, University of Leeds, 1998

(<http://www.scs.leeds.ac.uk/services/reports/1998.html>)],

has demonstrated that the Moving Finite Element (MFE) method may be applied to a class of parabolic partial differential equations (PDEs), for which a corresponding energy functional exists, in order to yield optimal steady-state solutions on optimal finite element meshes. The first half of this presentation will describe the main conclusions of this work and will clarify the exact nature of the optimality results.

The talk will then consider the further application of these results to a number of important elliptic PDEs. In particular, a “false-transient” MFE method will be discussed and the work of Miller and Baines, [K. Miller and M. J. Baines, Least Squares Moving Finite Elements, Oxford University Computing Lab. Report 98/06, Oxford University, 1998], on Least Squares Moving Finite Elements (LSMFE) will be described. It will be demonstrated that the theoretical results concerning particular parabolic equations may be applied to Miller and Baines’ false-transient LSMFE algorithm in order to prove that it can yield an optimal mesh when solving a very general class of PDEs.

The talk will conclude with some numerical examples which will illustrate how the LSMFE approach may be used to solve a number of test problems, including convection-diffusion equations, in a manner which will yield optimal solutions on optimal meshes. The potential importance of these techniques for use in general purpose adaptive finite element software will also be discussed.

A VISCOELASTIC HYBRID SHELL FINITE ELEMENT

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A hybrid large displacement thick-shell finite element is extended to allow for the calculation of viscoelastic stresses. Internal strain variables are introduced at the element's stress nodes and are employed to construct a time dependent constitutive model. First order ordinary differential equations relate the internal strain variables to the corresponding elastic strains at the stress nodes. Viscous stresses for the deformed shell element are computed from the internal strain variables using viscous moduli which are a fraction of the elastic moduli. In the formulation, a dissipative energy expression computed from the viscous stresses and strains is added to the nonlinear elastic variational statement. The nonlinear quasi-static viscous equilibrium equations for the shell element are then obtained. Previously developed Taylor expansions of the nonlinear elastic equilibrium equations are modified to include the viscous terms. A predictor-corrector time marching solution algorithm is employed to solve the quasi-static equations. The scheme simultaneously solves the nonlinear algebraic equilibrium equations with the Newton-Raphson method, and the differential equations for the internal strain variables with the trapezoidal method. A stair-step loading and unloading of an aircraft tire in contact with a frictionless surface is solved for a computational demonstration.

This work was supported by the Computational Structures Branch, NASA

ADAPTIVE METHODS FOR FINITE-TIME BLOWUP COMPUTATIONS

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An adaptive algorithm for the numerical simulation of finite-time blowup in the case of the 2-D Nonlinear Schrödinger equation is described. Results of numerical experiments are presented.

ON ROBUST PRECONDITIONING IN BEM WITH GRADED MESHES

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We discuss the nonstandard BEM formulations based on a product of the classical boundary integral operators recently proposed in [2]. The approach leads to the robust version of Galerkin-BEM on rather general graded meshes. In this way, we first precondition the continuous integral equation and then construct the Galerkin approximation for the transformed operator of the zero order. Kernels of the product integral operators are shown to have the low-order separable expansions yielding the data-sparse hierarchical approximations [1] of the Galerkin stiffness matrices. Finally, the fully robust scheme is obtained from the Galerkin equation by a simple diagonal scaling of the discrete L^2 -norm.

Our techniques may be applied in BEM (on the highly graded meshes) with the single layer, hypersingular and double layer potential operators for solving the elliptic equations of the second order. Relation to the interface-BEM (boundary integral equations in the nonoverlapping domain decomposition) will be also discussed.

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APPROXIMATION AND COMPLEXITY ANALYSIS FOR \mathcal{H} -MATRICES IN BEM/FEM APPLICATIONS

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A class of hierarchical matrices (\mathcal{H} -matrices) was introduced in [1] which are data-sparse and allow a matrix arithmetic of almost linear complexity. Several types of \mathcal{H} -matrices were considered in [1, 2, 3], which are able to approximate the integral and pseudodifferential operators in the case of quasi-uniform unstructured meshes.

In this talk, we discuss the consistency error and general complexity estimates for data-sparse hierarchical approximations to integral operators defined on domains/manifolds in R^d , $d = 2, 3$. The local kernel expansions by using both the Taylor and Legendre polynomials are analyzed. The resulting \mathcal{H} -matrices retain the approximation power

of the exact Galerkin scheme, on the one hand, and provide the asymptotically linear complexity (w.r.t. the problem size) for matrix-vector/matrix-matrix multiplications and matrix-inversion, on the other. Emphasis will be placed upon the sharp complexity bounds regarding the basic parameters of our techniques. Applications in the case of nonuniform meshes are also considered.

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FINITE ELEMENT METHODS FOR DIFFUSION EPIDEMIC MODELS WITH AGE-STRUCTURED POPULATIONS

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A numerical approximation is considered for a model of epidemiology describing age-dependent population dynamics with spatial diffusion. A finite difference method along the characteristic age-time direction is combined with finite elements in the spatial variable. Optimal order error estimates are derived for the approximation. Longtime behavior will be considered.

AN ERROR ESTIMATOR FOR THE FINITE ELEMENT ANALYSIS OF BEAMS

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This paper derives a Bank-Weiser type error estimator for finite element solutions to the thermoelastic equilibrium equations governing an Euler-Bernoulli beam. The technique involves the solution of a local problem over a single beam element using the residual as data. The estimator is proven to be asymptotically exact in the energy norm when the finite element solution is superconvergent at the connecting nodes. Numerical examples are presented to support the theory.

DISCONTINUOUS DOMAIN DECOMPOSITION METHODS WITH LAGRANGE MULTIPLIERS FOR ELASTICITY PROBLEMS

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In the last decade a lot of research has been carried out on iterative substructuring methods with Lagrange multipliers. In these methods the original domain is decomposed into nonoverlapping subdomains. The intersubdomain continuity is then enforced by Lagrange multipliers across the interface defined by the subdomain boundaries. A computationally very efficient member of this class of domain decomposition algorithms is the **Finite Element Tearing and Interconnecting** (FETI) method introduced by Farhat and Roux.

Several variants of the FETI method are considered and some new condition number estimates are given. Different popular scalings, e.g. as used for problems with composite materials, are analyzed.

The presented results are based on joint work with Olof Widlund, Courant Institute, New York University.

HIERARCHICAL ERROR ESTIMATES

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Hierarchical error estimates for finite element methods are based on higher order discretization of the discrete defect problem and localization by preconditioning techniques. Reliability of the resulting error estimate is equivalent to a saturation property. In this talk, we discuss the relations to other concepts like residual error estimates and some implications. Moreover, we present generalizations to obstacle problems and contact problems in linear elasticity.

HIERARCHICAL FINITE ELEMENT METHODS IN FRACTURE MECHANICS

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The numerical simulation of failure mechanisms is a highly complex and computationally challenging task. This is even more true for problems of significant engineering relevance. In order to enable simulation of failure initiation in situations where sufficient experimental data can not be found, it is necessary to enhance current *State-of-the-Art* models to incorporate low level mechanisms of fracture. The development of multiscale simulation capabilities in the context of high performance finite element methods is an important step in this direction.

The presentation will give a brief overview of multiscale methods in fracture mechanics, emphasizing on the importance of adaptive finite element methods. A framework for a fracture mechanics simulation system is outlined and certain performance aspects are addressed. Finally, the capabilities of the system are demonstrated on the application of adaptive multiscale methods to a creep rupture problem.

TETRAHEDRAL PARTITIONS OF ACUTE TYPE

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A tetrahedron is said to be of acute type if all six internal angles between its four faces do not exceed the right angle. For such a tetrahedron we prove that its triangular faces do not contain an obtuse angle.

A partition of a polyhedron into tetrahedra is said to be of *acute type* if all tetrahedra are of acute type. Such partitions play an important role in solving linear and nonlinear partial differential equations by the finite element method, since the corresponding stiffness matrices become diagonally dominant. This property enables us to derive a priori L^∞ -error estimates, to obtain discrete maximum principles, to employ the Monte Carlo finite element method, etc. We give several examples of acute type partitions. Then we discuss how to perform their acute type refinements.

Any triangle can be divided by midlines into four congruent triangles which are similar to the original one. However, the three-dimensional case is much more complicated. Note that a refinement of an acute type tetrahedron T "by midlines" produces 8 smaller tetrahedra which are not of acute type, in general. That is why we will

refine T in another way. Denote by S the centre of the circumscribed ball of T . If the interior of T contains S then we will decompose T into 24 acute type subtetrahedra whose common vertex is at S . Otherwise T will be decomposed into 18 or less smaller acute type tetrahedra. In the both cases each face F of T is subdivided into 4 or 6 right-angled triangles whose common vertex is the centre of the circumscribed circle to F . A numerical example will be presented.

CONVECTION DOMINATED COMPRESSIBLE FLOWS

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The basic idea for the discretization of conservation laws (or for the convective terms in convection dominated diffusion problems) in 1-D consists in solving local Riemann problems exactly or approximatively. It turns out that this can be generalized to finite volume schemes in multi dimensions on structured and in particular on unstructured grids. This is even true for higher order MUSCL type schemes. For scalar conservation laws in multi dimensions there are rigorous proofs for convergence to the entropy solution of these numerical schemes and error estimates. In this lecture we will present some recent results for a posteriori error estimates and how they can be used to local grid refinement.

Although there are nearly no proofs in the case of systems the generalized schemes work also very well. The AUSMDV Riemann solver turns out to be one of the best one. For the discretization of the convective terms for viscous flows we have the same numerical problems as for conservation laws. We will also show some applications of these schemes to complex (industrial) problems in 3-D, included parallelization and local grid refinement.

A MULTI-WELL PROBLEM FOR PHASE TRANSFORMATIONS

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We are concerned with the deformation process of a solid body composed of a thermoeelastic material undergoing stress-induced coherent martensitic phase transformations. A martensitic transformation is a first-order solid-to-solid phase change occurring in various crystalline solids, e.g. in the pseudoelastic *shape memory alloys* (SMA). This unusual behaviour is attributed to discontinuous changes in the crystal lattice of the high temperature phase, *austenite*, which possesses a greater symmetry and that of the low temperature phase, *martensite*, which may exist in many variants. Although the resulting microstructure of SMA is usually reversible under loading/unloading cycles, the latter induce hysteresis effects. Our approach is based on the minimization of the elastic energy [1, 2] and the second principle of thermodynamics [3]. More specifically, supposing that the material may appear in $N + 1$ preferred strain states: the parent phase (austenite) and N -variants of martensite, we postulate the Helmholtz free energy W_i ,

$$W_i(\mathbf{E}, \theta) = \frac{1}{2} (\mathbf{E} - \boldsymbol{\Gamma}_i) \cdot \mathbb{A}_i (\mathbf{E} - \boldsymbol{\Gamma}_i) + \varpi_i(\theta), \quad 1 \leq i \leq N + 1$$

where $\mathbb{A}_i = \mathbb{A}$ is the same elasticity tensor for each phase (variant), \mathbf{E} denotes the tensor of (small) strains, $\boldsymbol{\Gamma}_i$ is the transformation strain of i th phase, and θ is the temperature. For the free energy function of the mixture which is the multi-well piecewise quadratic functional $W(\mathbf{E}) = \min_{1 \leq i \leq N+1} \{W_i(\mathbf{E})\}$, we consider a homogenized free energy of the form

$$\widetilde{W}(\mathbf{E}, \mathbf{c}) = \frac{1}{2} (\mathbf{E} - \sum_{i=1}^{N+1} c_i \boldsymbol{\Gamma}_i) \cdot \mathbb{A} (\mathbf{E} - \sum_{i=1}^{N+1} c_i \boldsymbol{\Gamma}_i) + \sum_{i=1}^{N+1} c_i \varpi_i + \frac{1}{2} \sum_{i=1}^{N+1} \sum_{j=1}^{N+1} c_i c_j B_{ij}$$

where B_{ij} are material constants and c_i is the volume fraction of i th phase. We control the evolution of c_i by means of the second law of thermodynamics which leads to variational inequalities. Results of numerical experiments with the proposed formulation and the developed numerical algorithm will be presented.

Acknowledgement

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PARALLEL ITERATIVE SOLVERS FOR 3D MAGNETIC FIELD PROBLEMS

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Magnetic field problems are described by Maxwell's equations which reduce to $\operatorname{curl} \vec{H} = \vec{I}$ in the case of magneto-statics, where \vec{I} is the given current density and \vec{H} is the magnetic field strength. Introducing a vector potential \mathbf{u} for the magnetic induction \vec{B} ($\vec{B} = \mu \vec{H}$, permeability μ), the non-trivial kernel of the curl -operator causes the non-uniqueness of \mathbf{u} . That is why we re-formulate the problem as mixed problem in $H_0(\operatorname{curl}) \times H_0^1$ by adding some weak gauging condition. The resulting variational formulation can be discretized by mixed Nédélec and Lagrange type elements. The discrete problem can be reduced to a symmetric and positive definite system of equations in primal variables for which optimal multigrid preconditioners can be constructed.

The parallelization of the sequential algorithm is based on a non-overlapping distribution of the finite element mesh. This provides automatically distributed finite element matrices and a parallel conjugate gradient (cg) algorithm can be realized easily. Major challenges arise in our case from mixed discretizations (nodal- and edge-based degrees of freedom), block-smoothers and coarse-grid solvers required by the multigrid preconditioner. In order to overcome these problems we have developed an object-oriented software concept.

We will present applications of 3D magnetic field problems. Parallel results are obtained on a ORIGIN 2000.

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ADAPTIVE MULTI-LEVEL FEM SIMULATION FOR COUPLED FIELD PROBLEMS

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This poster presents algorithms and software tools for the finite element simulation of coupled field problems. Especially, we consider the coupling of static and dynamic mechanical and magnetic problems in 3d.

The implemented solvers are based on multi-level preconditioners on adaptively refined hierarchical meshes. We stress the importance of robust components. This means, the discretization error, the iteration number of the solver, and the quality

of the a posteriori error estimator must not degenerate as certain parameters form geometry (e.g. thin walled structures) or materials (e.g. Poisson ration) become bad.

We explain, how we implemented a toolbox of components like bilinear-forms, pre-conditioners etc., which can be used in an overall solution procedure for the coupled problem. The presentation includes also topics from geometric modeling, mesh generation, problem description and visualization.

A POSTERIORI ERROR ESTIMATION FOR ANISOTROPIC TETRAHEDRAL FINITE ELEMENT MESHES

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Many physical problems lead to boundary value problems for partial differential equations, which can be solved with the finite element method. In order to construct adaptive solution algorithms or to measure the error one aims at reliable *a posteriori* error estimators. Many such estimators are known, as well as their theoretical foundation.

Some boundary value problems yield so-called *anisotropic* solutions (e.g. with boundary layers). Then anisotropic finite element meshes can be advantageous. However, the common error estimators for isotropic meshes fail when applied to anisotropic meshes, or they were not investigated yet.

For *rectangular* or *cuboidal* anisotropic meshes a modified error estimator had already been derived. In this paper error estimators for anisotropic *tetrahedral* or *triangular* meshes are considered. Such meshes offer a greater geometrical flexibility.

For the Poisson equation we introduce a residual error estimator, an estimator based on a local problem, several Zienkiewicz-Zhu estimators, and an L_2 error estimator, respectively. A corresponding mathematical theory is given. For a singularly perturbed reaction-diffusion equation a residual error estimator is derived as well. The numerical examples demonstrate that reliable and efficient error estimation is possible on anisotropic meshes.

The analysis basically relies on two important tools, namely anisotropic interpolation error estimates and the so-called bubble functions. Moreover, the correspondence of an anisotropic mesh with an anisotropic solution plays a vital role.

BOUNDARY ELEMENT ANALYSIS OF THE CONTACT CONDITIONS BETWEEN CERAMIC-COATED MECHANICAL COMPONENTS

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The reliability and useful life of mechanical components such as steel bearings can be improved by using protective overlay coatings of more resistant materials. This protection is fundamental to reduce wear at the surface of these non-conforming contact components where high localised stress concentrations are usually found.

This paper presents a boundary element analysis of the stress distribution in ceramic-coated mechanical components under contact conditions. The physical, non-conforming contact between components such as spherical bearings, or between bearings and flat substrates, makes the problem geometrically nonlinear; therefore, an iterative procedure of solution is required.

An efficient axisymmetric boundary element formulation has been developed for this purpose using appropriate fundamental solutions given in terms of complete elliptic integrals. The numerical formulation incorporates features such as subregions modelling and a fast iterative solver based on *LU* decomposition and the Sherman-Morrison-Woodbury formula.

Numerical results to be presented include parametric studies in which the variables investigated are the friction conditions, coating thickness and the ratio between the Young's modulus of ceramic/steel.

SOLVING SHORT WAVE PROBLEMS USING SPECIAL FINITE ELEMENTS

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In order to model the wave potential using finite elements, it is usual to discretize the domain such that there are about ten nodal points per wavelength. However, such a procedure is computationally expensive and impractical if the waves are short compared to the dimensions of the problem. The goal is to be able to model accurately with few elements problems such as sonar and radar. Therefore we seek a new method in which the discretization of the domain is more economical.

In the present method, the complex potential is expressed in terms of the wave amplitude with respect to several chosen directions. And instead of modelling the potential using many finite elements per wavelength, we model the wave amplitude using finite elements containing many wavelengths per nodal spacing. The aim is to solve short wave problems using a coarser mesh.

The problem of interest deals with the diffraction of an incident plane wave by a rigid cylinder. It is formulated by the Helmholtz equation, Neumann boundary condition

and the radiation condition at infinity. The resulting elementary matrices obtained from the Galerkin-Bubnov formulation contain oscillatory terms and are evaluated using high order Gauss-Legendre integration. The number of integration points and the number of the chosen directions to obtain the solution depend on the given wave number of the problem.

The results already obtained show that the method is very promising. Several wavelengths can be contained within each finite element. If the numerical procedure is improved and the problem process is parallelised then the method could allow very fast simulations compared to the usual finite element method.

MATHEMATICAL SCIENTIFIC COMPUTING TOOLS FOR 3D MAGNETIC FIELD PROBLEMS

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3D magnetic field problems are challenging not only because of interesting applications in the industry but also from the mathematical point of view. Usually, technical 3D magnetic field problems are characterized by complicated interface geometries with possibly moving parts (e.g. rotating parts), large coefficient jumps, non-linearities, singularities, and the necessity of calculating the exterior magnetic field. In practice, the aim of the simulation is often the optimization of the magnetic device we are dealing with. In order to handle such kind of technical magnetic field problems, it is not sufficient to have a fast Maxwell solver and optimizer, but also a geometry modeller, an advanced 3D mesh generator, mesh handling and refinement methods, parallelization tools, and postprocessing tools including advanced visualization techniques are required.

We will present such pre- and postprocessing tools, especially adapted to adaptive multilevel methods used in the solver and the optimizer. Of course, the heart of our magnetic field problem solver environment FEPP is an adaptive multilevel Maxwell solver. In the magnetostatic case, the Maxwell solver is based on special mixed variational formulations of the Maxwell equations in $H_0(\text{curl}) \times H_0^1(\Omega)$ and their discretization by the Nédélec and Lagrange finite elements. Combining this with an adaptive nested multilevel preconditioned iteration approach, we obtain an optimal solver with respect to the complexity. This is confirmed by the results of numerical experiments for academical problems and real life applications as well. We also propose a concept for coupling finite elements with boundary elements. Coupled finite and boundary element schemes are especially suited for problems where it is necessary to take into account the exterior magnetic field.

For the parallelization, two different strategies have been developed. The first approach uses a thread-based implementation that is especially suited for shared memory parallel computers such as the ORIGIN 2000. It is highly efficient if small numbers of processors are used. The second concept is based on distributed data algorithms and has been developed for massively parallel computers and workstation clusters.

More information on the problem solver environment FEPP and on the presented results can be obtained from the homepage
<http://www.sfb013.uni-linz.ac.at> of the special research project (SFB) "Numerical and Symbolic Scientific Computing" that is supported by the Austrian Science Foundation (FWF).

FINITE ELEMENT MODELLING OF THE PLUG ASSISTED THERMOFORMING PROCESS

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In the production of food packaging using the plug assisted pressure thermoforming process it is desirable to optimize costs and product properties through efficient distribution of material. Typically in industry conditions for forming are obtained by trial and error which can be very inefficient. The principle aim of this work was to develop a numerical model of the process that would provide quantitative predictions in a convenient way, so that trial and error methods could be eliminated. Modelling was carried out using a commercial finite element package and the model encompassed both 2D axisymmetric and more complex 3D geometry. Developing a material model that accurately describes the complex non-linear viscoelastic material behaviour was a difficult task. A large part of this problem was finding material properties at conditions comparable to the actual process. Material behaviour was simulated using a simple viscoelastic model based on data obtained from various material tests. Inclusion of heat transfer was also shown to be of great importance in producing an accurate model of the process. A conduction model based on Fourier's law was implemented in the model. Predictions from the model were in good agreement with actual thermoforming tests. Further work is required to improve the material model with the aid of extensive material tests at different temperatures and strain rates.

DISCRETE LEAST SQUARES FOR HYPERBOLIC EQUATIONS AND SYSTEMS INCORPORATING MESH MOVEMENT

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A finite volume method is presented for steady advection equations and conservation laws on unstructured meshes incorporating mesh movement. The method can substantially improve the resolution of sharp features (contacts, shocks) by solving on an optimal mesh. Results are presented for a number of steady state test problems, including scalar advection and the shallow water equations in 2-D.

A great deal of effort is currently being put into mesh refinement near shocks using mesh subdivision, but similar improvements in resolution can also be obtained much more cheaply by minor adjustments to the mesh. A requirement is a criterion for mesh adjustment, parallelling the monitor functions used in mesh subdivision.

We consider a descent approach using a least squares measure of the residual. The procedure is to interleave mesh adjustment steps between steps of a least squares type scheme. For scalar equations there is a close relationship with the method of characteristics. For systems of equations additional linearisation is necessary to make progress: however, encouraging results are obtained for flows in channels governed by the shallow water equations. A discontinuous least squares method for shocked flows is described which uses the nonlinear shock jump residual to adjust the mesh.

HP-ADAPTIVE FINITE ELEMENT METHODS FOR VISCOELASTIC FLOW CALCULATIONS

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An adaptive high-order finite element method is used to calculate the creeping flow of a viscoelastic fluid around a sphere falling in a cylinder. No corner singularity appears in such a flow, but from a quite complex flow field, one predicts the drag correction factor.

Most of the early numerical simulations have been performed with the upper-convected Maxwell model. This model seemed to have the simplest constitutive equations exhibiting most typical viscoelastic effects. However, it has been found that the flow of such fluid is one of the most difficult to simulate among the available constitutive equations, as it may generate more numerical difficulties than apparently more complicated differential models. The upper-convected Maxwell model is therefore often used as a benchmark model for numerical methods. Hence, a huge amount of numerical results is now available for this fluid. The *classical mixed formulation* of the corresponding viscoelastic problem is given by :

Find (τ, u, p) such that

$$\begin{aligned} \tau + \lambda \nabla \cdot \tau - 2\mu D(u) &= 0, \\ -\nabla p + \nabla \cdot \tau &= 0, \\ \nabla \cdot u &= 0, \end{aligned}$$

where u is the velocity field, p is the pressure, τ is the viscoelastic extra-stress tensor, μ is the viscosity, λ is the relaxation time of the fluid and $D(u)$ is the rate of deformation tensor. The symbol ∇ denotes the upper convected derivative given in a steady flow by :

$$\nabla = (u \cdot \nabla) \tau - \nabla u^T \cdot \tau - \tau \cdot \nabla u.$$

Accuracy and robustness of the results are demonstrated by p -convergence analysis and by comparison with reference results. Hence, our calculations with high-order interpolations may be considered as reference results for this problem. Several stabilize formulations (MIX, EVSS, AVSS, DEVSS, DAVSS) are analysed and compared. Error

estimation and adaptivity allow us to derive optimal discretizations for each formulation. We observe that both suitable formulation and discretization are critical to obtain a valid prediction.

ON THE FOURIER-BOUNDARY ELEMENT METHOD FOR ELLIPTIC PROBLEMS WITH EDGE SINGULARITIES

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Let Γ be a closed polygonal curve in the plane. We consider the three-dimensional transmission or interface problem

$$-\Delta u = 0 \text{ in } (\mathbb{R}^2 \setminus \Gamma) \times (0, \pi); \quad u = f \text{ on } \Gamma \times [0, \pi], \quad u(x, y, 0) = u(x, y, \pi) = 0.$$

We prove the following facts:

- With (f_ℓ) the Fourier coefficients of f , the transmission problem has a unique variational solution $u(x, y, z) = \sum_{\ell=1}^{\infty} u_\ell(x, y) \sin(\ell z)$, where each Fourier coefficient u_ℓ solves the two-dimensional transmission problem

$$-\Delta u_\ell + \ell^2 u_\ell = 0 \text{ in } \mathbb{R}^2 \setminus \Gamma; \quad u_\ell = f_\ell \text{ on } \Gamma. \quad (1)$$

- Each u_ℓ is the single-layer potential $u_\ell(x, y) = V_\ell(x, y; q_\ell)$, $(x, y) \in \mathbb{R}^2 \setminus \Gamma$, of the Helmholtz operator in (1), the density q_ℓ being the unique variational solution of the boundary integral equation

$$V_\ell(x, y; q_\ell) = f_\ell(x, y), \quad (x, y) \in \Gamma. \quad (2)$$

- The operator $q_\ell \mapsto u_\ell$ is continuous with constant independent of ℓ .

- The density q_ℓ is decomposable into regular and explicit singular parts.

Regarding the numerical treatment, Problem (2) is considered first. Let q_ℓ^h in the space X_h of piecewise constant functions be the solution of the associated boundary element method. Despite the presence of corner singularities, a suitable refinement of the mesh size h leads to the optimal convergence below.

- The function $u^h := \sum_{\ell=1}^{\infty} u_\ell^h(x, y) \sin(\ell z)$, where $u_\ell^h(x, y) := V_\ell(x, y; q_\ell^h)$, is a semi-discrete approximation of u such that $\|u - u^h\| = O(h)$.

- For a fixed integer $N \geq 1$, the truncated Fourier series

$$u^{h,N}(x, y, z) := \sum_{\ell=1}^N u_\ell^h(x, y) \sin(\ell z)$$

satisfies $\|u - u^{h,N}\| = O(h + N^{-1})$.

FINITE ELEMENT METHOD WITH OPTIMAL BASIC FUNCTIONS

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In 1978 year author proposed of the optimal finite element method (OFEM). In this method finding of the basic functions, parameters and knots of the elements from condition of the minimization of the functional of energy (see,for example, O. Lytvyn, Extended nonlinear interpolation and solution of boundary value problems, Differential equations.Minsk,1983, v.19, N3, pp.508-515. -russian). In this talk survey and some new results of the numerical realization this and other schemes OFEM for the elliptic differential equations 2nd and 4th orders (rectangular and triangular elements,include elements with one curvilinear side) is given .

Apparently, this method with well known versies $h-p$ FEM ,adaptive schemes FEM (with effective methods a posteriori error estimation) and optimal meshes may be in further important instruments of investigators for solution real complex boundary value problems.

Below main idea OFEM is given. Let we consider next boundary value problem

$$Au(x) = f(x), x = (x_1, \dots, x_n) \in \Omega, \partial^s u(x)/\partial \nu^s = 0, x \in \partial\Omega$$

$\Omega \subset R^n$ - bounded domain (for simplicity,let Ω -rectangular polyhedron: its boundary $\partial\Omega$ consists with faces what is parallel to co-ordinate flats) ; ν - normal to $\partial\Omega$; $f(x) \in L_2(\Omega)$; A - selfadjoint elliptic operator of the order $2m$:

$$Au = \sum_{|\alpha| \leq m} (-)^{|\alpha|} D_x^\alpha (a_\alpha(x) D_x^\alpha u), \alpha = (\alpha_1, \dots, \alpha_n), |\alpha| = \sum_{k=1}^n \alpha_k, D_x^\alpha u = \frac{\partial^{|\alpha|} u}{\partial x_1^{\alpha_1} \dots \partial x_n^{\alpha_n}}$$

Let $x_k = x_{k,i_k}, i_k = \overline{1, N_k}, k = \overline{1, n}$ be a partition of the domain Ω into elements $\Pi_i = \bigcap_{k=1}^n [x_{k,i_k+1}, x_{k,i_k}] \subset \Omega, \pi = \{i = (i_1, \dots, i_n) : x^i = (x_{1,i_1}, \dots, x_{n,i_n}) \in \Omega \setminus \partial\Omega\}; E_{n,m} = \{\alpha = (\alpha_1, \dots, \alpha_n) | \alpha_k = \overline{0, m-1}; k = \overline{1, n}\}; \Delta_{k,i_k} = x_{k,i_k+1} - x_{k,i_k}; u_{i,\alpha}(i \in \pi, \alpha \in E_{n,m})$ -unknown constants; $h_{i,j,k,\alpha_k}(t_k)$ ($j \in \{0, 1\}$) - unknown basic functions with properties

$$h_{i,j,k,\alpha_k}(t_k) \in C^{2m}[0, 1], h_{i,j,k,\alpha_k}^{(s)}(\gamma) = \delta_{s,\alpha_k} \delta_{0,\gamma} (s, \alpha_k = \overline{0, m-1}; \gamma \in \{0, 1\});$$

S_N - of the space of the functions $u_{\pi,m}(x)$ of the form:

$$u_{\pi,m}(x) = \sum_{l \in \pi} \sum_{\alpha \in E_{n,m}} u_{l,\alpha} \prod_{k=1}^n \bar{h}_{i,k,\alpha_k}(x_k), \text{supp } \bar{h}_{i,k,\alpha_k}(x_k) = [x_{k,i_k-1}, x_{k,i_k+1}]$$

$$\bar{h}_{i,k,\alpha_k}(x_k) = \begin{cases} h_{l,0,k,\alpha_k}((x_{k,i_k} - x_k)/\Delta_{k,i_k-1})(-1)^{\alpha_k} \Delta_{k,i_k-1}^{\alpha_k}, & x_{k,i_k-1} \leq x_{k,i_k}, \\ h_{l,1,k,\alpha_k}((x_k - x_{k,i_k})/\Delta_{k,i_k}) \text{Delta}_{k,i_k}^{\alpha_k}, & x_{k,i_k} \leq x_{k,i_k+1}. \end{cases}$$

Unknown constants $u_{i,\alpha}$ and basic functions $h_{i,j,k,\alpha_k}(t_k)$ finding from the conditions: $\partial J(u_{\pi,m})/\partial u_{r,\beta} = 0, \delta_{h_{r,j,k,\beta_k}} J(u_{\pi,m}) = 0, r \in \pi, \beta \in E_{n,m}, j \in \{0, 1\}, k = \overline{1, n}$, where $\delta_h J(\dots, h, \dots)$ - variation of the functional J with respect of function h . These is a systems of Rietz's and system nonlinear integro-differential equations. The

method's of its numerical solution is given. This approach may be realized with simultaneous minimization of the functional J with respect to parameters x_{k,i_k} , $k = \overline{1, n}$, $x^{(i)} \in \Omega$ of the mesh.

A UNIFIED INVERSE FINITE ELEMENT STRATEGY FOR PARAMETER IDENTIFICATION OF COUPLED PROBLEMS

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The proposed algorithm for parameter identification of coupled problems within a finite element setting is applied to three specific examples of coupled problems:

- 1.) Firstly, we consider geometrically linear Terzaghi-Biot type fluid-saturated porous media. Thereby, the set of equations is conceptionally split into a solid and a fluid problem, which are essentially the consequences of the balance of linear momentum and the balance of mass, respectively, for a two phase mixture together with some simplifying assumptions [1]. The basic independent field variables of the coupled field problem are the displacements and the excess pore fluid pressure.
- 2.) Secondly, we consider the coupled initial boundary value problem of a geometrically linear gradient damage model in the framework of continuum mechanics. Following [2] the set of equations is conceptionally split into an equilibrium problem – as a consequence of the balance of linear momentum – and a non-local equivalent strain problem – as a consequence of a Taylor-Series for the non-local equivalent strain variable. This approach is motivated by the need to avoid mesh dependence of the classical local theory. The basic independent field variables of the coupled field problem are the displacements and the non-local equivalent strain variable.
- 3.) Thirdly, we consider the coupled initial boundary value problem within geometrically linear thermo-elasticity coupled to damage. Here, the set of equations is conceptionally split into an equilibrium problem – as a consequence of the balance of linear momentum – and an energy balance equation – as a consequence of the first and second law of thermodynamics, see e.g. [3]. The basic independent field variables of the coupled field problem are the displacements and the temperature.

For all kinds of problems a least-squares functional consisting of experimental data and simulated data is minimized, whereby the latter are obtained with the Finite-Element-Method. In this way non-uniformness of the associated field quantities during the identification process is possible, and the strategy allows parameter identification based on in-situ experiments. In order to improve the efficiency of the minimization process, a gradient-based optimization algorithm is applied, and therefore the corresponding sensitivity analysis for the associated coupled problem is described in a systematic manner. For illustrative purpose the performance of the algorithm is demonstrated for a number of numerical examples based on synthetic data.

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MORTAR ELEMENT METHOD FOR BOUNDARY ELEMENT DISCRETIZATIONS OF ELLIPTIC PROBLEMS

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The mortar finite element method is an example of a non-conforming method which can be used to decompose and re-compose a domain into subdomains without requiring compatibility between the meshes on the separate components. We apply this method to boundary elements for the hypersingular integral integration on polyhedral surfaces. This integral equation corresponds to the Neumann boundary problem for the Laplacian. We generalize the recent stability and convergence results of Seshaiyer and Suri to 3D-BEM.

For practical 3D problems with edge and corner-edge singularities mortar interfaces pass through singularities.

Even in these cases our numerical results for hp mortar BEMs show that the mortar method behaves as well as conforming boundary element methods.

**EFFICIENT SOLUTION ALGORITHMS FOR
SIMULTANEOUS MULTIPLE FREQUENCY ANALYSIS
OF EXTERIOR ACOUSTICS PROBLEMS**

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In this paper we address the development of efficient Krylov-subspace algorithms for the simultaneous solution of exterior problems over multiple frequencies and with multiple sources. The work is based on the use of finite elements in the computational domain and the Dirichlet-to-Neumann (DtN) map for the non-reflecting boundary condition. In broad terms, the approach is based on three principal developments:

1. For the DtN map, a new algorithm for the efficient computation of matrix-vector products.
2. A new algorithm for simultaneous solution over multiple frequencies based on a new variant of the block quasi-minimal residual (BL-QMR) algorithm for simultaneous solution of a family of shifted linear systems.
3. A new algorithm for the efficient computation of partial fields at multiple frequencies using Padé extrapolation-based reduced-order models.

The DtN and modified DtN boundary conditions have the advantage that they can be made arbitrarily accurate but have the disadvantage that they are nonlocal and couple all degrees of freedom on the boundary. The computational and storage costs associated with the DtN formulation can become large enough to limit its use in conjunction with Krylov subspace methods. An efficient new algorithm to compute matrix-vector products, based on the structure of the DtN kernels, has been developed which dramatically reduces storage requirements while being highly efficient for computing matrix-vectors products. A matrix-free DtN condition is also recovered as a special case. Connections between the DtN map and discrete Fourier transforms in two dimensions and discrete spherical transforms in three-dimensions are established to provide further improvements in efficiency. An efficient preconditioning approach that utilizes an SSOR-type splitting is also described.

An extension of the BL-QMR algorithm has been developed that enables the simultaneous solution of a family of shifted linear systems for essentially the cost of one solution. This development along with the algorithm for the DtN maxtrix-vector product noted above, provides the framework for solving multiple linear systems over a range of frequencies at a significantly reduced cost, potentially providing several orders of speed-up. The application of the shifted BL-QMR algorithm to an exterior radiation problem has demonstrated its potential for significantly accelerating multiple frequency solutions. Solutions at 200 frequencies in the range $0 < ka < 20$ were computed using only six factorizations and about 400 back-solves, in place of 200 factorizations and 400 back-solves needed for a sequential solution.

Many problems of significant practical interest can be cast as partial-field problems,

including, for example, determination of far-field pressures or pressures at a few specified locations. A novel framework for obtaining such partial field solutions can be based on highly accurate Padé approximation-based reduced-order models. The main idea behind this approach is to formulate a frequency-dependent transfer function that relates given input loads to a chosen number of “modal” coefficients of the pressure field on the DtN surface, which become the unknowns when the pressure is represented using the corresponding surface harmonics. The transfer function is reformulated by exploiting the outer-product form of the DtN condition. The relation between a novel Lanczos-type process for multiple starting vectors and matrix-valued Padé approximations is used to replace the transfer function, which is of a large size, by a “reduced-order” matrix, which is its matrix Padé approximant. Once the “modal” coefficients are available on the DtN surface, the far-field pressures can be computed using the analytical solution of the exterior DtN problem or the surface Helmholtz-Kirchhoff integral theorem. The reduced-order modeling technique enables fast simultaneous computation of far-field pressures for multiple frequencies at only a fraction of the cost involved in solving the full system of linear equations.

BOUNDARY ELEMENT METHODS AND SOUND RADIATION – HOW TO CREATE EXPLICIT FREQUENCY DEPENDENT MATRICES

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The use of explicit frequency dependent matrices as in finite element methods has not really been established in boundary element methods yet. The Dual Reciprocity Method (DRM) and the Particular Integral Method (PIM) may be applied to construct explicit frequency dependent matrices. These have been tested for the solution of interior problems in structural acoustics. However, a formulation for the exterior problem using DRM or PIM have not been found yet. In this paper, the author wants to discuss ideas and ways to apply the Particular Integral Method to solve the acoustic boundary value problem for open domains either using suitable admittance boundary conditions or creating a special formulation for exterior problems.

COUPLING PROCEDURES IN PARTITIONED METHODS FOR FLUID STRUCTURE INTERACTION

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Partitioned methods for fluid-structure interaction, i.e. where different codes are used for the different physical domains, are investigated. For the sake modularity and manageability of the resulting software architecture, it is highly desirable to build coupled codes out of simpler modules.

The physical and mathematical requirements are formulated and analysed with respect to the information to be transmitted for the coupling procedure. Depending on the method for spatial and temporal coupling, certain desiderata for the coupling interface emerge. Some recent proposals for such interfaces are analysed in this respect.

Additional requirements arise from the need to use fast multi-level solvers within each physical domain and across the different physical domains.

RAPID MESH METHODS FOR SOLVING INHOMOGENEOUS BIHARMONIC INTEGRAL EQUATIONS

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We present rapid fourth order accurate methods for solving inhomogeneous biharmonic equations of the type that arise in low Reynolds number problems in fluid mechanics. The methods use integral equation formulations based on complex variables, and make use of fast finite difference methods for evaluating the volume integrals and Cauchy integrals that arise in the formulations. Numerical results are presented for experiments on a variety of geometries.

A FULLY DISCRETE BEM-FEM METHOD FOR THE EXTERIOR STOKES PROBLEM IN THE PLANE

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The BEM-FEM method for exterior Stokes problems in R^2 has been first introduced by Sequeira [A. Sequeira, The coupling of boundary integral and finite element methods for the bidimensional exterior steady Stokes problem, *Math. Meth. in the Appl. Sci.*, 5, 1983, pp. 356–375]. She used the so called “one boundary integral equation approach” given in Johnson-Nedelec [C. Johnson, J. C. Nedelec, On the coupling of boundary integral and finite element methods, *Math. of Comp.*, 35, 1980, pp. 1063–1079] for the Laplace equation. This procedure consists in dividing the exterior domain into a bounded inner region and an unbounded outer one by introducing an auxiliary common boundary. Next, the integral representation of the solution in the unbounded part is used to deduce a non-local condition on the auxiliary boundary for the problem in the inner region.

Our purpose is to present a new numerical scheme for this coupling method. We follow [S. Meddahi, An optimal iterative process for the Johnson–Nedelec method of coupling boundary and finite elements, *SIAM J. Numer. Anal.*, 35, 1998, 1393–1415] and use a parametric representation of the artificial boundary to represent all terms on this boundary via periodic functions. This leads to a formulation which is equivalent to the classical one, offering some additional advantages in the numerical treatment.

For the discretization of the problem in the inner domain we use curved triangles, which induces the use of a curved stable finite element for the Stokes problem. For this purpose, we generalise the mixed element introduced in [C. Bernardi, G. Raugel, Analysis of some finite elements for the Stokes problem, *Numer. Anal.* 26, 1989, pp. 71–79]. We give the error analysis of the corresponding Galerkin scheme and present a family of full discretizations of the complete set of equations by using simple quadrature formulas. We show that the resulting scheme is well posed and retains the optimal order of convergence.

INTEGRAL EQUATION METHODS FOR SCATTERING BY ROUGH SURFACES

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We consider the problem of wave scattering by infinite one-dimensional rough surfaces. An ansatz is made for the scattered field employing either the free-field Green's function or a fundamental solution for a half-space. This leads to an integral equation for which we propose a theoretical Nyström method that converges super-algebraically provided the boundary is smooth enough. The method is applied in the case of a periodic surface and numerical results are presented. Subsequently, the method is developed further by introducing an iterative scheme in which the kernel is approximated by a Taylor or Chebychev series expansion. We will present a stability theorem and show some numerical results including a comparison with the diffraction grating case above.

HP-FEM FOR SINGULARLY PERTURBED REACTION-DIFFUSION EQUATIONS IN CURVILINEAR POLYGONS

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The hp -version of the finite element method (hp -FEM) is applied to a singularly perturbed reaction-diffusion model problem in polygonal domains. For piecewise analytic input data it is shown that the hp -FEM can lead to *robust exponential convergence* on appropriately designed meshes, i.e., the rate of convergence is exponential and does not deteriorate as the perturbation parameter tends to zero. These meshes consist of one layer of needle elements of width $O(p\varepsilon)$ at the boundary (here, p is the polynomial degree employed and ε measures the length scale of the boundary layer) and geometric refinement toward the vertices of the domain.

We will highlight the key ingredients of the convergence analysis and illustrate the robust exponential convergence with numerical examples.

COMPUTER AIDED DESIGN OF PREFORMS FOR INJECTION STRETCH BLOW MOULDING

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The most common process to produce PET soft drink containers is injection stretch blow moulding. Simulations of the process have been performed using the Abaqus finite element package. The temperature distribution of the preform and the process conditions for a variety of bottles were found and input into each simulation.

A non-linear viscoelastic material model based on the molecular makeup of PET developed by Buckley [Buckley, P; Jones, D: Polymer, Vol. 37, No.12, pp. 2403-2414, 1996] has been used to model the PET behaviour during forming. The resulting thickness distributions from the simulation were compared with those obtained experimentally, which showed that the simulations were sufficiently accurate to be useful in optimising preform shape and processing conditions.

A methodology has been developed to use the material distribution produced by the simulation to predict the shelf life of the container. Software has been written which accesses the stretch ratios and thickness of each element of the formed model and from these properties the shelf life can be predicted.

A POISSON PRESSURE APPROACH TO FINITE ELEMENT STRESS ANALYSIS OF NEARLY INCOMPRESSIBLE MATERIALS

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It is well known that the equal-order Galerkin finite element approach to stress analysis of nearly incompressible materials in either irreducible or mixed formulation may produce highly oscillatory pressure solutions [O. C. Zienkiewicz and R. L. Taylor, The Finite Element Methods: Basic Formulations and Linear Problems, Volume 1, McGraw-Hill, London, 1989]. Even if mixed, lower order pressure interpolation is employed there are still cases where numerical difficulties are encountered [R. L. Sani et al, The Cause and Cure of the Spurious Pressures Generated by Certain FEM Solutions of the Incompressible Navier-Stokes Equations: Part 1, International Journal for Numerical Methods in Fluids, Vol. 1, 17-43, 1981].

This paper presents an alternative approach to finite element stress analysis based on the possibility to formulate a separate Poisson equation for pressure. So far, the Poisson pressure approach has been considered only as an attractive alternative formulation of the incompressible viscous flow equations [P. M. Gresho, Incompressible fluid dynamics: Some fundamental formulation issues, Annu. Rev. Fluid. Mech., Vol. 23,

413–453, 1991] which requires special care in the implementation of boundary conditions [S. Hassanzadeh et al, Finite Element Implementation of Boundary Conditions for the Pressure Poisson Equation of Incompressible Flow, Int. J. Numerical Methods in Fluids, Vol. 18, 1009–1019, 1994]. The aim of this paper is to propose the extension of the Poisson pressure approach also to the problems of nearly incompressible elastic and viscoelastic materials. Special emphasis is put on the formulation of corresponding finite element statements and the implementation of derived boundary conditions.

The main advantage of the Poisson pressure approach in stress analysis is a possibility to employ the standard equal-order interpolation finite element methods with no constraints imposed on the interpolation orders for the displacement (velocity) and pressure as in the mixed formulations. The accuracy and stability of the proposed methodology has been tested in numerical experiments involving stress analysis problems related to the thermal oxidation and thin film deposition processes in the semiconductor fabrication technology.

4-NODE QUAD AS DIRICHLET TYPE OF BOUNDARY VALUE PROBLEM

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The properties of the 4-node quad are investigated in an analytical way, where a finite element is considered as a plane elastic boundary value problem with prescribed boundary displacements (Dirichlet problem). Of the 8 eigen modes of this element 3 are rigid body modes and 5 deformation modes. The deformation modes consist of 3 with uniform deformation modes and 2 bending modes, the so-called hour-glass modes. For the uniform deformation modes the solution of the the corresponding boundary value problem is trivial, leaving the hour-glass modes as the only challenging ones. The analytical solution of the latter problem has been achieved using extended Fourier series expansion of the displacement field. The calculation of the coefficients could only be done using numerical methods. From a geomechanics point of view the most interesting aspect of the result is that the solution is only non-unique in the Poisson ratio range $\sim 0.6 < \nu < \sim 0.9$, while the sufficient condition of uniqueness covers the parameter range $\nu \leq 0.5$ and $\nu > 1$. In this context it should be noted that the equivalent elastic parameters of dilative materials like dense sand can leave this parameter range of well-posedness as well.

ANALYSIS OF VIBRATIONS OF WETTED ELASTIC STRUCTURES BY FE-BE-METHOD

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The practical analysis of vibrations of wetted elastic structures is a complex procedure. It will be often advantageous to combine an elastokinetic FE-model for the structure and the boundary element method for the fluid in the numerical treatment of this interaction problem. The discussed procedure is based on a boundary integral formulation of the potential problem of an incompressible and nonviscous fluid for internal and external problems. The discretisation is realized by a boundary element collocation method with discontinuous interpolation of variable order. Finite boundary elements with an analytical integration scheme and infinite elements with partially analytical or fully numerical integration are used. The infinite elements allow the effective modeling of an unbounded fluid domain. The influence of the fluid is considered in the dynamic FE-equations of the structure by added masses. The procedure also allows to analyze problems with several separate fluid domains simultaneously as well as structures wetted on both sides. The procedure provides an improvement compared with the method of Lewis which is still frequently used in practice.

TIME DOMAIN UNSTRUCTURED GRID APPROACH FOR ELECTROMAGNETIC SCATTERING IN PIECEWISE HOMOGENEOUS MEDIA

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We consider the development of a 2D and a 3D capability for the time domain simulation of scattering of electromagnetic waves in piecewise homogeneous media using unstructured triangular or tetrahedral grids. It is assumed that the waves are produced by a source in the far field and a scattered field formulation is employed, with the governing equations considered in a dimensionless form. For such simulations, the computational domain is bounded by a closed external boundary and may contain material interfaces, thin resistive sheets and perfectly conducting boundaries. It is assumed that this computational domain is represented by a general unstructured grid of linear triangular or tetrahedral elements, constructed by using a mesh generator which includes a multi-domain meshing capability [1]. A variational formulation of Maxwell's curl equations is employed and the approximate solution is obtained by advancing in time by an explicit two-step finite element Taylor-Galerkin procedure[2, 3], which is notionally second order accurate in both time and space. All boundary and interface conditions are satisfied in a weak sense only and this requires the duplication of nodes which are located at material interfaces before the solution process begins. In this approach, the solutions on either side of an interface are coupled by the boundary integral terms which arise in the variational formulation. These boundary integral terms are evaluated by using a local characteristic decomposition at the boundary [4].

A number of examples will be presented to demonstrate the numerical performance of the proposed procedure. The examples will involve the scattering of plane waves by configurations of simple geometrical shape, such as cylinders or spheres, as this will allow comparison to be made between the numerical results and the exact analytical solutions.

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APPLICATION OF FINITE ELEMENT METHOD TO PERIODIC BLOOD FLOW

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This work describes the results obtained from analytic, numerical and experimental models of periodic blood flow in a rigid axi-symmetric tube. The main part of the work involves a Computational Fluid Dynamic model to investigate the nature of periodic blood flow. A numerical model is particularly useful in this application since it gives detailed magnitudes, locations and duration of shearing forces, both on the vessel wall and in the flow itself. This level of detail would be very difficult to obtain from an experimental model alone. The potential benefits of improved understanding of physical blood flow are significant in the control and treatment of a wide range of cardiovascular conditions. The model simulates blood flow past both smooth and periodic surfaces, representing the human coronary artery. A very fine grid is used since the problem is axi-symmetric and the flow domain is relatively small. A periodic pressure boundary condition composed of four harmonics was used to drive the flow. The Navier-Stokes equation for an incompressible, transient flow was solved using a Finite Element method. Particle tracking was used to visualise the paths of individual blood components. For smooth surfaces the velocity field was compared to the equivalent analytic solutions, which show good agreement. The flow over periodic surfaces shows regions of recirculations in the depressions into which blood components become partially trapped during the forward flow. During a brief period of reverse flow, the particles in the recirculation washed out and are ejected into the mainstream of the flow. Also the distribution of wall shear stress histories are presented showing the effect on the vessel wall. These characteristics may play an important part of blood flow induced thrombosis particularly soon after the introduction of a vascular implant.

COUPLING BOUNDARY INTEGRALS — FINITE ELEMENTS IN MAXWELL EQUATIONS

Jean-Claude Nédélec and Habib Ammari

Several techniques of coupling between integrals equations and finite elements has been implemented by several authors. One of the very first work on this subject was made by V. Levillain in his thesis. He obtain nice numerical results, but was not able to give any proof of convergence. We will prove that the techniques he has been using, are in fact stable and converging. We will use different decomposition techniques and prove some Gårding inequalities.

FLOW BALANCING IN EXTRUSION DIES FOR THIN WALLED THERMOPLASTIC PROFILES

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The rheological design of extrusion dies must consider the flow developed through the die channel and the influence of the post-extrusion phenomena. Currently there are several software available for modelling the flow in extrusion dies [1, 2, 3, 4, 5]. Despite being powerful modelling tools, they only consider some of the relevant phenomena and the design process is not fully automatic. Therefore, there is still a need to develop an algorithm integrating all the relevant aspects in order to enable the automatic die design optimisation [6, 7].

For the particular case of non-axisymmetric profile extrusion dies, the flow must be balanced in order to guarantee uniform melt velocity at the die exit contour [8], avoiding distortions promoted by draw-down. The difficulty to achieve flow balancing increases when thin flow channels are considered, since minor changes in the channel geometry / operating conditions may promote relevant changes in the flow distribution.

This work focuses on the flow balancing problem, considering the extrusion die shown in Figure 1., and modelling the flow with the Polyflow [1] finite element based software. The calculations are fully three-dimensional and non-isothermal. The effect of changes in the channel geometry (adapter and land), operating conditions (throughput, melt inlet temperature and die surface temperature) and mesh refinement are illustrated.

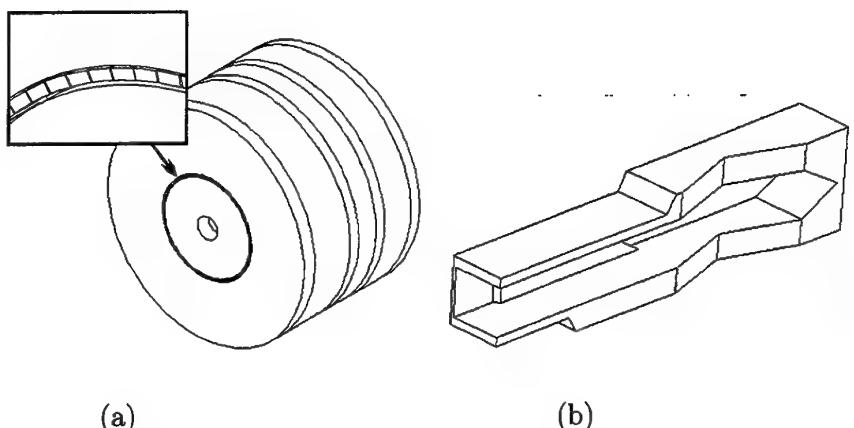


Figure 1. Extrusion die (a) and correspondent channel considered in the flow modelling (b)

This study will help to select the most relevant factors to be considered in the automatic balancing of profile extrusion dies, as a part of a global optimisation die design algorithm.

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ESTIMATION OF MODELING AND APPROXIMATION ERROR IN MULTISCALE MODELS OF HETEROGENEOUS MATERIALS

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We consider a class of highly complex, boundary value problems in solid mechanics characterized by models of heterogeneous materials exhibiting multiple spatial scales. Such models are encountered in analysis of composite materials and of microstructural effects on service life and strength of materials. The resolution of the solution, and its gradients for problems, with such irregular coefficients is a computational problem of enormous size and complexity. In the present study, we explore the concept of adaptive modeling, coupled with adaptive meshing. We derive upper and lower bounds of errors in quantities of interest produced by both modeling error, due to replacing the real microstructure in a heterogeneous material with that of a homogenized material; we also obtain upper and lower bounds of errors in the finite element approximations of quantities of interest. These estimates include the effects of pollution errors in both local modeling error and local approximation error. Having error estimates, we then construct adaptive techniques that simultaneously adapt the model, the mesh, and local spectral order. Simulations of the behavior of heterogeneous materials in significant engineering applications are considered.

LOCAL ERROR ESTIMATORS AND ADAPTIVITY FOR ELASTIC PROBLEMS

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Local error estimators get increasing importance in engineering practice when certain quantities are of interest in small subdomains only; those quantities are, e.g., stresses at notch- and crack tips or energy release rates as criteria for crack propagation.

Due to results of BABUŠKA ET AL. [1], CIRAK & RAMM [2], RANNACHER ET AL. [4] and OHNIMUS ET AL. [3] local residual type error estimators are available, and some research codes have been developed for elastic problems. A special task is the effective description of far field influence, the so-called pollution error, represented by Green's influence functions.

In the present paper, both local residual (primal) type and dual type quantitative error estimators are derived using special enhanced test spaces and solving separated local Neumann problems. Both for the proper local error as well as for the global pollution error by discretizing Green's function. This is done for adaptive computations of local displacements, local stresses and stress resultants as well as for Rice integrals in fracture mechanics which is a matter of current research. The upper bound property of the estimators is pointed out.

Previous results show that the effectivity index is considerably improved by using local Dirichlet problems even in the case of residual type error estimators. The dual local estimators by the PEM (Posterior Equilibrium Method), i.e. dual type error estimators yield competitive results and they are advantageous in case of locking problems.

Also local estimators for non-linear elastic problems are in progress and might be implemented into the lecture.

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SOME ADVANCED COMPUTATIONAL STRATEGIES FOR THE MODELLING OF FORMING PROBLEMS

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Introduction

This paper discusses some issues in the computational treatment of non-linear problems which have arisen out of the necessity to solve various classes of industrial forming problems. Although the applications considered are taken from a range of commercial sectors, the principal numerical challenges are largely common. The main issues relate to the implementation of advanced constitutive models under conditions of finite strain elastic and inelastic deformations, element methodology for incompressible behaviour, mesh adaptivity strategies and equation solution procedures for large scale problems.

Constitutive Modelling

A basic requirement of the computational modelling of non-linear material behaviour under finite strain conditions is the consistent linearisation of the discretised equations. The development of consistent tangent operators becomes progressively more difficult with increasing complexity of the constitutive models employed. For example, simulation requirements for industrial operations involving powder compaction and soft solids processing has lead to the introduction of pressure dependent constitutive laws of the Gurson and crushable foam types. Problems associated with the efficient computational implementation of such models within a finite strain setting are discussed.

A main development concerned with modelling frictional contact phenomena is the description of a model particularly suited to coated sheet materials. A model is described which is based on the plasticity theory of friction in which a hardening variable is introduced to represent the dependence of friction on the degree of relative sliding between the tool and workpiece. Attention will also be given to the development of a computational procedure for predicting tool wear.

Adaptivity with Evolving Geometries

A general feature encountered in the finite element simulation of forming operations, such as forging or deep drawing, is that the optimal mesh configuration changes continually throughout the deformation process. Therefore, the introduction of adaptive mesh refinement processes is crucial for the solution of large scale industrial forming problems, which necessitates (i) a remeshing criterion, (ii) specification of an appropriate error estimation criterion, (iii) development of a strategy for adapting the mesh based on the error distribution and (iv) automatic mesh generation tools.

For forming problems, in which the geometric changes are usually large, the decision to update the finite element mesh is invariably based on *element distortion* parameters and the role of error estimation is then to decide the element size distribution in the new mesh. In view of its fundamental importance to inelastic problems of evolution through the second law of thermodynamics, an error estimation strategy based on the *plastic dissipational functional* and the *rate of plastic work* is introduced. For problems involving non-linear behaviour, and plastic deformation in particular, issues related to the transfer of variables from the old mesh to the new mesh are crucially important

for preserving the robustness and convergence properties of the finite element solution. Problems in this area become especially acute when deformations are large, resulting in evolving geometries as is the case in forming simulations. When mapping from the old to new mesh, (i) Consistency with the *constitutive equations*, (ii) The requirements of equilibrium, (iii) Compatibility of the state transfer with the *displacement field* on the new mesh, and (iv) Compatibility with evolving *boundary* and *loading* conditions must be satisfied. A transfer strategy for large strain elasto-plastic problems is described in which the current displacement field and the plastic part of the deformation gradient corresponding to the previous converged solution is employed for state transfer.

Explicit Solution Strategies

The excessive computational times associated with implicit quasi-static solutions of forming problems has lead to the extensive use of explicit time integration procedures. Typically, for large scale 3D problems solution by the explicit method can be accomplished at least one order of magnitude faster than the corresponding implicit analysis. However, inertia effects have no significant influence in most forming operations and efficient explicit solution of these essentially quasi-static problems depends on choice of artificial values for parameters such as the material mass and process speed. The paper discusses issues related to the efficiency and accuracy of explicit solution procedures for forming problems and also illustrates the role of mesh adaption strategies.

Element Methodology

A fundamental requirement for bulk forming simulations is the use of appropriate elements which can model the incompressible nature of the plastic flow without exhibiting locking behaviour. The tendency of the solution to lock, that is provide overstiff solutions with poor stress representation, becomes more predominant when large deformations are involved, as is the case in all forming operations. In addition to producing unacceptable stress fields within the workpiece, this also leads to a poor representation of surface tractions and hence to incorrect prediction of contact/friction conditions between the tools and workpiece. The paper discusses some of the more popular strategies employed to overcome these difficulties. One effective solution to this problem is offered by the F-bar element in which a multiplicative split of the deformation gradient is employed to enforce the incompressibility constraint. The element is free from hourgassing defects, exhibits a relatively large bowl of convergence and is especially suitable for adaptivity applications.

Equation Solution and Parallel Processing

The ever increasing need to solve large scale industrial problems by an implicit approach demands that advances be made in equation solution strategies. As equation systems extend beyond a certain size (of the order of 20,000 dof), direct solvers become increasingly inefficient and iterative solvers offer the most natural approach to solution. Currently, the most promising candidates are Conjugate Gradient (CG) or multi-grid techniques. CG methods are commonly employed, with various pre-conditioning strategies utilised to improve the conditioning of the equation system (e.g. Jacobi, Incomplete Cholesky, etc.). Considerable promise is also offered by multi-grid methods; in which the problem is first solved on a coarse mesh to pre-condition the equation system for subsequent solution by CG on a finer mesh. Issues related to the solution of large scale problems by iterative solvers are discussed.

The rapid emergence of parallel processing hardware, even at the multi-processor workstation level, necessitates consideration of solution methods for forming problems by concurrent computational methods. In this respect domain decomposition techniques offer efficient parallel implementation and can be utilised on both shared and

distributed memory computers. Furthermore, they are applicable to both implicit and explicit solution algorithms. Issues which require detailed consideration are load balancing, memory allocation and data communication, with a need to provide generic solution strategies in addition to solutions for specific architectures. Implementation issues are discussed, including the treatment of evolving contact conditions.

PARALLEL DOMAIN DECOMPOSITION PROCEDURE BASED ON PRIMAL MIXED FINITE ELEMENT METHOD

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A parallel domain decomposition iterative procedure for primal mixed finite element method for second order elliptic equations is proposed and analyzed. Robin transmission conditions are used to pass information from a subdomain to its neighbors. A convergence of the iterative algorithm is proved. Numerical examples are presented. The method is applicable to the steady-state drift-diffusion model of semiconductor devices.

MULTILEVEL METHODS FOR DOMAIN DECOMPOSITION WITH LOCALLY REFINED MESHES

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In this talk, I will consider the application of multilevel methods in conjunction with non-overlapping domain decomposition methods for problems with refined meshes. I will consider both the problem of constructing H^1 bounded extensions as well as that of preconditioning the so-called Schur Complement system. I will show that both problems can be solved using multilevel methods. This give rise to a domain decomposition preconditioners with a uniform rate of convergence for problems with local grid refinement.

**SIMULATION OF DENTAL IMPLANTS UNDER CYCLIC
LOADING USING A VORONOI TESSELLATION BASED
FRAME MODEL OF TRABECULAR BONE AND *P* VERSION
FINITE ELEMENTS FOR COMPACT BONE**

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In this paper, we describe new models for the computer simulation of endosseous dental implants. Most current finite element models of such systems have used simplifications such as isotropy, homogeneity, perfect contact and simple axial loads in order to make the computations tractable. Here we use a Voronoi tessellation based frame structure to model the porous cellular structure of trabecular bone. We also relax the assumptions of static loading and use cyclic loads. The use of Voronoi cells enables the modeling of the variable porosity of the trabecular bone in different parts of the bone. Initial microcracks are assumed to exist in the structure and grow according to the Paris law with each loading cycle. The initial crack distribution is governed by a random beta distribution function. Once the crack reaches a predefined critical size, the trabecular is extracted from the structure, thereby weakening it and lowering the overall secant modulus of the structure. When the overall modulus shows a 10% drop, the structure is assumed to fail. The frame model of trabecular bone is then coupled with a continuum *p* version finite element model of the cortical bone and embedded implant. The coupling between the two models is enforced with both strong and weak continuity of the displacement fields. We present several example results obtained by our analyses that appear to agree well with qualitative empirical observations of implant failure.

AFEAPI: ADAPTIVE FINITE ELEMENTS APPLICATION PROGRAMMERS INTERFACE

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Parallel adaptive hp finite element methods(**FEM**), in which both grid size h and local polynomial order p are dynamically altered are the most effective discretization schemes for a large class of problems. The greatest difficulty in using these methods on parallel computers is the design of efficient schemes for data storage, access and distribution. Benefits derived from such methods may be completely lost without good schemes for these. Further, most application developers lack both the resources and the skills to develop such complex codes. We describe here the development of a comprehensive infrastructure, AFEAPI, that addresses these concerns. AFEAPI will provide a simple base for users to develop their own parallel adaptive hp finite element codes. It will be responsible for the dynamic data structure, mesh partitioning and redistribution and optionally solution of the large irregularly sparse systems of linear equations generated in these schemes. It can also be easily customized for different applications. User customization will comprise of providing appropriate routines for generating element stiffness matrices, material data and optional error computation routines.

The principal ideas underlying AFEAPI are the use of a simple data addressing scheme using keys based on geometric location of element/node centroids on a "space filling curve" and integration with mesh partitioning and dynamic load balancing schemes that use the same ordering. Dynamic hashing schemes and balanced trees are used to store and access the distributed unstructured data efficiently. Example two and three dimensional applications and performance data will be presented.

"INDUSTRIAL STRENGTH" SOLVERS
- DOMAIN DECOMPOSITION, ITERATIVE
AND MULTI-LEVEL SUBSTRUCTURING

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The focus of this paper is the development of a class of robust iterative solvers that can reliably solve irregularly sparse and often poorly conditioned linear systems arising from adaptive and higher order finite element methods. Iterative solvers ($O(N^2)$ operation count) especially those making use of multi-level and multi-grid ideas have been long seen as more efficient than standard direct solvers($O(N)^3$ operation count). This is particularly true on parallel computers where parallel factorization is slowed down by heavy communication requirements. However, these *faster* iterative solvers often do not converge in a reasonable number of iterations, negating all advantages of such solvers. This is a situation that is often seen in problems with adaptive and higher order meshes, large mesh distortion and or widely differing material properties. In past work, on these methods we have developed iterative substructuring based solvers and coarse grid hierarchical preconditioners that are quite efficient for model elliptic problems. For such problems, we have proved that they have condition numbers that grow at rates that are polylogarithmic in the mesh discretization parameters. However, on more complex problems such efficiencies are not obtained. In related work we have also developed a multi-level substructuring type solvers based on a good fill-reducing ordering using a space-filling curve passing through the element centroids. This solver is very robust, but not as efficient as the iterative substructuring solvers.

We report here the development of hybrid solvers that combine the advantages of both by automatically switching from one algorithm to the other, depending on the problem, to produce robust solvers that work reliably on a large class of problems. The solver starts with a substructuring on the lowest levels (bubble and edge function degrees of freedom) that are local to a processor, and switches to a preconditioned iterative solver at a level of the hierarchy that requires access to non-local data. The preconditioner is a very coarse grid and diagonal blocks corresponding to the remaining degrees of freedom. If the solver exhibits difficulty in converging, we expand the definition of the preconditioner to include more and more degrees of freedom until we reduce to the multi-level substructuring solver described earlier. Further, since the choice of which solver is more efficient on a multi-processor architecture is dependent on the relative costs of computation and communication it is possible to tune these solvers to particular machine architectures by selecting the number of levels of substructuring to use.

OVERLAPPING SCHWARZ PRECONDITIONERS FOR UNSTRUCTURED SPECTRAL AND *HP*-ELEMENTS

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Overlapping Schwarz methods provide optimal domain decomposition preconditioners for the iterative solution of elliptic problems discretized with h-version finite elements and finite differences. In this talk, we will show that this is also the case for spectral elements and hp-version finite elements. If the basis employed is nodal, which is often the case for structured spectral elements based on Gauss-Lobatto-Legendre (GLL) quadrature, then we can construct overlapping methods using either generous overlap (a whole spectral element) or minimal overlap (one or a few GLL points in each direction). For unstructured spectral elements employing tetrahedral and prismatic elements in addition to hexahedral elements, a nodal basis is not yet known and therefore we propose to use overlapping methods with generous overlap. Numerical results for scalar elliptic problems in two and three dimensions with the CFD research code Nektar show that the condition number of the preconditioned iteration operator is bounded independently of the spectral degree and the number of elements. This result holds for the additive and multiplicative versions of the preconditioner. It is also possible to eliminate implicitly the degrees of freedom belonging to the interior of each element and apply the overlapping method to the resulting Schur complement. We are able to prove this optimal bound only in the case of structured hexahedral meshes and tensor product basis functions, but the numerical results presented show that the result holds for general unstructured meshes as well. This is joint work with Tim Warburton of Oxford University, UK.

DOMAIN DECOMPOSITION FOR MULTIPHASE FLOW: INTERFACE COUPLING OF DIFFERENT NUMERICAL AND PHYSICAL MODELS

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It is generally believed that the coupling of different models may be the only way to achieve progress in modelling and simulation of problems with complex geometry and physics. Currently many highly specialized algorithms and codes exist which can perform the local tasks in an already optimal or nearly optimal manner. The coupling of these specialized codes is the focus of our paper.

In industrial practice many codes have been coupled together in a loose fashion for example by using interface values delivered by one code as boundary values for the next time step of another code. Our Multiblock Multi-Model framework allows for tight coupling. The interface values are our unknowns at every time step. Their values are sought iteratively with a domain decomposition procedure which stops when the conservation of the quantities in question has been satisfied to a given tolerance level. In our applications to multiphase flow in subsurface, the quantities matched at interface are pressures, and the conservation of mass across the interface is achieved by iterating the difference in the phase fluxes to zero (or desired tolerance).

The issues involved in the Multiblock Multi-Model framework can be split loosely into five categories. First the Multiblock approach gives the mathematical foundation to nonmatching grids on the interface, which is achieved with the use of mortar spaces for mixed finite elements. Next comes the interface solver which currently uses the inexact Newton-Krylov algorithm and the choice of preconditioner which is subject to many constraints but is crucial to efficiency of the whole procedure. Another interesting problem arises when different numerical algorithms like fully implicit around the wells and sequential in the far field are coupled which may possibly use different time stepping and implicit / explicit boundary values.

The coupling of multiphysics adds another dimension to the above. For example some part of the subsurface reservoir is completely saturated with water and can be handled efficiently by a single phase code or sequential two phase code, while the adjacent part will have some hydrocarbon phases and wells which will be simulated by a fully implicit two or three phase code. Of course, the domain decomposition algorithm here must ensure that the phase boundaries do not cross the interface between the subdomains. It is worth mentioning that, while physically and numerically legitimate, the use of the three phase code can take several times longer to simulate the given two phase case, and is computationally obsolete for the single phase.

Last but not least comes the question of implementation issues measured in many years of developing specialized models and coupling them using the Multi-Model approach versus computational complexity measured in computer cycles burnt on multiple processors.

In the paper we present our results obtained as joint effort of the research group at Center for Subsurface Modelling at TICAM, UT Austin.

3D MAGNETIC FIELD ANALYSIS IN A PERMANENT MAGNET BRUSHED MOTOR

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The permanent magnet brushed motor is a simple electric machine widely used in automotive industry and in the industry for home appliances, too. The proper evaluation of the magnetic field and its analysis is a part of each motor design procedure or performance analysis. The object for which the magnetic field is calculated is a 2-pole permanent magnet brushed motor with rated data: power 80W, voltage 20V, speed 450 rpm and torque 1.6 Nm. The segmental permanent magnets mounted on the stator frame with an overlap angle of 135° are made of anisotropic barium ferrite with remanent magnetic flux density of 0.38 T and with coercitive field strength of -254 kA/m.

The calculation of the magnetic field and the necessary data for an analysis of the magnetic field distribution in the permanent magnet brushed motor is provided by an own computer program package called FEM-3D, based on the 3D Finite Element Method. In order to realise a numerical solution of the magnetic field distribution it is necessary to carry out a corresponding mathematical modelling of the permanent magnet brushed motor in its 3D domain.

In the pre-processing stage of the package FEM-3D, the program performs an efficient mesh generation in the three dimensional domain of the motor, using the concept of *macro elements*. The accepted shape is curved rectangular prism with 20 nodes and six sides (faces). This shape is considered to be the most suitable for the geometrical configuration of electrical machines. The subdivision into *finite elements*, shaped as 6 noded, 5 sided triangular prism is carried out fully automatically. The macro elements are chosen to be as least different as possible, and repetitive as much as possible. All different macro elements are named *pilot-macro elements*. By rotating and/or shifting them the whole domain under consideration is covered (overlaid) with macro elements, resulting from the repeating and the symmetry of the motor configuration.

The program package FEM-3D, based on the concept of Weighted Residuals, performs a non-linear iterative calculation of the Poasson's or Laplace's equation, and the output data are the values of the magnetic vector potential and its components $\mathbf{A} = \{A_x, A_y, A_z\}$ in every node of the discretized domain. Having the permanent magnets with an anisotropy along z-axis inside the motor, the corresponding mathematical model suitable to the FEM application in the 3D domain is derived. Due to the lamination of magnetic core the different magnetic reluctivities along the three co-ordinate axes are taken into consideration, as well.

By execution of the program FEM-3D the results of the magnetic vector potential values in the nodes of the finite element mesh covering the whole three dimensional domain of the permanent magnet brushed motor are obtained. These values can be used to plot the magnetic field distribution in different layers of the three dimensional domain of motor. The calculation of the magnetic field distribution starts at rotor position $\beta = 0^\circ$ (when there is a rotor slot in front of the permanent magnet neutral axis) and

at rated current load $I_n = 6A$. Calculations of the magnetic field are proceeded for different rotor displacements $\beta = 5^\circ$, $\beta = 10^\circ$, $\beta = 15^\circ$, $\beta = 20^\circ$ and for different current loads starting from $I = 0 A$ up to $I_n = 6 A$. On the basis of the results obtained, a deepened analysis of the magnetic field distribution in the 3D domain of the permanent magnet DC brushed motor will be done.

In the full paper, some of the electromagnetic and electromechanical characteristics of the permanent magnet DC brushed motor, calculated in the post-processing stage of FEM-3D application, will be presented and fully analyzed, too. The results will be compared with the experimentally obtained ones.

SEMI-LAGRANGIAN FINITE VOLUME METHODS FOR VISCOELASTIC FLOW PROBLEMS

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Recently, there has been considerable interest in solving viscoelastic problems in 3D particularly with the improvement in modern computing power. In many applications the emphasis has been on economical algorithms which can cope with the extra complexity that the third dimension brings. Storage and computer time are of the essence. The advantage of the finite volume formulation is that a large amount of memory space is not required. Iterative methods rather than direct methods can be used to solve the resulting linear systems efficiently.

The SIMPLER algorithm is used as the basis of the finite volume technique described in this paper together with a semi-Lagrangian treatment of the convective terms. The standard finite volume approach for problems in computational fluid dynamics suffers from restrictions on the size of the time step due to stability considerations. This restriction is not so severe when particle tracking (Lagrangian) methods are used. However, the unrestricted movement of the points in a Lagrangian formulation introduces a new set of difficulties. Semi-Lagrangian methods combine the advantages of fixed grids inherent in Eulerian methods with modifications to treat the convective terms using particle tracking methods.

The hyperbolic nature of the constitutive equation is responsible for many of the difficulties associated with the numerical simulation of viscoelastic flows. Many techniques introduce some form of upwinding in order to obtain numerical solutions at high values of the Deborah number. In some finite volume techniques artificial diffusion has been added to the constitutive equation. The Semi-Lagrangian approach described here is a natural way of treating the convective terms in the constitutive equation without resorting to these techniques.

Numerical results are presented for the viscoelastic flow of an Oldroyd B fluid through a planar 4:1 contraction. Particular emphasis is given to the convergence and stability of the method and the development of vortex structure with increasing Weissenberg number.

SIMULATION OF THREE-DIMENSIONAL FLOW OF BLOOD IN THE CORONARY ARTERIES AROUND STENOSES BASED ON THE FINITE ELEMENT METHOD

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The paper deals with a specific application of computational fluid dynamics to the field of cardiovascular diseases, namely the three-dimensional simulation of the blood flow in the epicardial arteries around stenoses (narrowing of these arteries), based on the finite element method.

The most important function of the cardiovascular system is to transport the substances involved in metabolic processes taking place in the cells (tissues and organs). A relatively small but very important part of the systemic circulation is the coronary circulation which is responsible for a sufficient supply of blood to the myocardium. The coronary blood flow can be reduced by diffuse atherosclerotic plaques and especially by stenoses (narrowing) in the epicardial arteries. It is thus very important to provide physicians (especially coronary surgeons) with simulation models of the coronary blood flow.

The three-dimensional blood flow in a stenosed epicardial artery can be formalised in terms of partial differential equations (three-dimensional continuity equations and three-dimensional Navier-Stokes equations) which we have solved numerically using the finite element method. We used the software package "FIDAP" (Fluid Dynamics Analysis Package) of Fluent, Inc. which is a complete, integrated computational fluid dynamics (CFD) package for simulating fluid flow. We generated a mesh composed of hexahedra by using a semi-automatic method which requires some interaction with the user. The method used is based on the so-called multiblock approach. In this approach, the user subdivides the flow domain into several suitable blocks. The shape of the blocks must be such that an automatic (local) mesh generation method can be applied to each block.

The finite element method allows the computation of an approximate solution, provided that we are able to specify the essential boundary conditions. It is logical to assume "no slip" conditions at the wall of the stenosed artery and "natural" boundary conditions (normal stress is equal to zero) at the outlet (as the contribution of viscosity to the normal stress is relatively small, "natural" boundary conditions force the pressure to be close to zero at the outlet). It is also logical to assume a paraboloid velocity profile at the inlet. However, it is difficult to arrive at a quantitative specification of the boundary conditions at the inlet, since our three-dimensional model describes the flow in a particular stenosed artery that is only one of many sections of the coronary system. We have solved this problem by using a coarse model of the entire cardiovascular loop and a detailed lumped parameter models of the coronary network.

The simulation results which will be presented comprise velocity, pressure and shear stress in the flow domain and shear stress in the vessel wall. The finite element analysis of our fluid flow problem produces a wealth of numerical data. However, long lists of numerical data are difficult to analyse. Therefore, we will represent our simulation results as "fishnet" surface plots, contour plots, diagrams, and other graphics which

are adequate to analyses.

SMOOTH APPROXIMATION FOR THE VERIGIN-MUSKAT PROBLEM AND SAFFMAN-TAYLOR INSTABILITY

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The purpose of this talk is to show that the Buckley-Leverett system

$$\kappa P_t + \operatorname{div} \mathcal{F} = 0, \mathcal{F} = -M(s, x, t) \nabla_x P \quad (1)$$

$$s_t + F'(s) \mathcal{F} \nabla_x s = \varepsilon \Delta \Phi(s) \text{ in } Q_T = \Omega \times (0, T)$$

can be considered as a smooth approximation of the Verigin-Muskat free boundary problem. Here either $\kappa = 1$ or $\kappa = 0$, Ω is a bounded domain of \mathbf{R}^n , $n = 1, 2, 3$, with smooth boundary $\partial\Omega = \partial\Omega^+ \cup \partial\Omega^-$, $\partial\Omega^+ \cap \partial\Omega^- = \emptyset$, \mathcal{F} is the filtration velocity of the fluid,

$$M(s; x, t) = (K_* + L_*) f_1(s) + (K_* - L_*) f_2(s)$$

is the mobility coefficient, the functions $K_*, L_* \in C^\infty(\overline{Q}_T)$ are such that $K_* > L_*$ and f_1 and f_2 are dimensionless functions which are called relative phase permeabilities.

In fact we show three different free boundary problems which can obtained as limits of the Buckley-Leverett system as $\varepsilon \rightarrow 0$: the standard Verigin-Muskat problem is one of them. Discontinuous limiting saturations are obtained as solutions of a quasilinear first order equation with a discontinuous coefficient on the free boundary. In order to prove a local in time convergence result, we construct formal asymptotic expansions which approximate solutions of the Buckley-Leverett system and whose zeroth order term satisfy one of the limiting free boundary problems. We shown that the standard equation of the Buckley-Leverett system allows one to select the initial data of the sharp-fronted displacement that is stable displacement.

As well known the classical solution of limiting problems does not exists in the case $n > 1$ in general. But the classical solution always exists for $n = 1$. This fact allows one to construct formal asymptotic expansions in the case $n = 2$. This asymptotic solution approximates the small perturbation of the solution of the system (1), for which the solution one-dimension limiting problem is obtained by the passage to the limit. The perturbation should be periodic with respect to the another plane variable. This plane example explains the formation of Saffman-Taylor instability.

HIERARCHICAL MODELLING USING H- AND P-VERSION FINITE ELEMENT APPROXIMATIONS

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The finite element approximation is by nature a projection of the mathematical solution of a given problem onto the space spanned by its basis functions. An approximation can be improved by using an enrichment of the approximation space and it has turned out in many applications, that a hierarchical enrichment is advantageous from the theoretical as well as the practical point of view. We shall use the same concept of hierarchical enrichment for the definition of the mathematical problem to be solved, in order to improve the approximation of the underlying physical problem.

This duality of model hierarchy and finite element hierarchy can be used in various fields of application. A classical method having been used for decades in finite element analysis, the use of singular shape functions to approximate the behaviour near singularities, can be interpreted as a special case of hierarchical enrichment. It is also possible to use a combination of h - and p -versions for simulating structural problems with different inherent length scales. Other examples are hierarchical enrichments of models and approximation for a transition from two- to three-dimensional problems, or from linear to non-linear behaviour.

We will give in our paper a general outline of the basic ideas of this method, show various numerical examples for different applications and discuss the efficiency of our approach.

THE DUAL-WEIGHTED RESIDUAL METHOD FOR ERROR CONTROL AND MESH ADAPTATION IN FINITE ELEMENT METHODS

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We present a general concept of a posteriori error estimation and mesh size control in finite element Galerkin discretizations. The method is based on weighted a posteriori error estimates for functionals of the solution which are obtained by global duality arguments. The computed adjoint solutions contain quantitative information about the global dependence of the error quantity on the local cell residuals and can be used for guiding the mesh refinement process. This approach is particularly useful in cases where the local residuals do not control the local error, e.g., in the presence of global pollution effects, strongly varying coefficients and multi-physics processes. This is illustrated by some examples from fluid mechanics and astrophysics.

A POSTERIORI ERROR ESTIMATION AND MESH ADAPTATION FOR FINITE ELEMENT MODELS IN ELASTO-PLASTICITY

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A new approach to a posteriori error estimation and adaptive mesh design based on techniques from optimal control is presented for primal-mixed finite element models in elasto-plasticity. This method uses global duality arguments for deriving weighted a posteriori error bounds for arbitrary functionals of the error representing physical quantities of interest. In these estimates local residuals of the computed solution are multiplied by certain weights which are obtained by solving a linearized global dual problem numerically. The resulting local error indicators are used in a feed-back process for generating economical meshes. This approach is developed for the Hencky and Prandtl-Reuss models in linear-elastic perfect plasticity.

SHAPE OPTIMIZATION FOR LARGE DEFORMATION IN ELASTOPLASTICITY

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Although large deformation problems in elastoplasticity belong to classical areas of mathematical modelling, this subject is not discussed very often in a context of shape optimization. The main difficulty featuring optimization of elasto-plastic bodies arises as a consequence of nondifferentiability of the state problem solution with respect to design variables. In this paper we present some aspects of using the nonsmooth approach to the sensitivity analysis for a case of finite deformation elastoplasticity.

To this date a number of mathematical models in finite elastoplasticity exist that are well suited for the return-mapping solution procedure. However, the models based on existence of an intermediate stress-free configuration, which belong to the most challenging ones, are not easy to adopt for computing the sensitivity calculations and would require some essential changes in the existing approach recently used for treating the case of infinitesimal theory of elastoplasticity.

In this paper we shall consider a range of elastoplastic deformation for which the assumed additive decomposition of the total strain can be justified. Under this restriction of applicability we can develop a mathematical model which arises as a direct extension of the model published in [E. Rohan, J. R. Whiteman: Shape optimization of elasto-plastic structures and continua. (*to appear in Comp. Meth. Appl. Mech. Eng.*)].

Based on the total Lagrangian framework the state problem formulated in strain space involves variational inequalities associated with the isotropic hardening law and with a frictionless contact interaction. After discretization using linear finite elements in space and the implicit integration scheme in time the state problem can be expressed in the form of a sequence of nonsmooth equations. The sensitivity analysis can be computed adopting the adjoint equation method for time dependent problems.

As an application we consider an impact of a beam-shaped 2D solid with a rigid obstacle. The contact boundary can be shaped by design variables associated with the control polygon of a B-spline curve. Two optimal design problems are tested: minimization of stresses in plastic zone and minimization of contact stresses. For numerical optimization we use a version of the bundle method which requires to be supplied with an accurate (sub)gradients of the objective function.

FINITE ELEMENT MODELLING OF SMOOTH MUSCLE TISSUES

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The first step in modelling a biological tissue is to define a constitutive law which is “flexible” enough to correspond with the essential data obtained from experiments. Smooth muscle tissues belong to the most complicated biological materials due to a complex microstructure which strongly affects their behaviour. The characteristic property of all muscle tissues is the capability of generating force, or deformation as a response on the electrochemical stimulation. In that context an adequate mathematical model should approximate the muscle’s behaviour in both the resting and active states.

In this paper we present our efforts to treat smooth muscle tissues as composite type structures consisting of the incompressible hyperelastic matrix and of a fibreous network. The latter comprises collagen viscoelastic fibres and muscle fibres which being activated can produce force and, thus, reinforce the material. Due to properties of collagen fibres we consider them to have no resistance in compression. Thus, using so called “tension-only-properties” the collagen fibres stiffen the structure as the deformation progresses. Further we assume that at any point in the material the fibres of the k -th preferential direction occupy a volume fraction which does not change with time.

In our approach we consider two coupled subproblems involving the displacement field $\underline{u} = (u_1, u_2, u_3)$, the hydrostatic pressure p and the tension τ in fibreous phase. The deformation subproblem is defined within a total Lagrangian framework using the mixed formulation with the incompressibility condition. Viscoelasticity of fibres is embedded in variational inequalities formulated in terms of τ to differ between tension and compression of the structure. In order to approximate the problem we use 3D mixed finite elements with discretisation of p and τ associated with the pressure nodes. For generating solutions to the nonlinear system at each time level the Newton method steps are being alternated by projection steps successively. We also discuss the identification of material parameters involved in the model, which is based on the sensitivity analysis of the state problem. Some numerical results with identification of the muscle tissue at the resting state are presented.

NONCONFORMING METHODS FOR MAXWELL EQUATIONS WITH APPLICATION TO MAGNETOTELLURICS

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We present a collection of global and domain-decomposed nonconforming mixed finite element procedures to solve the 3D forward problem in magnetotellurics. The method deals with Maxwell's equations as a first order system of partial differential equations; first order absorbing boundary conditions are used on the artificial boundaries, in order to diminish undesired reflection effects.

Results obtained on a IBM SP/2 parallel supercomputer at Purdue University are shown. The accuracy of the numerical method is verified by comparison with numerical solutions provided by well known methods.

VARIABLE ORDER PANEL CLUSTERING

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We present a new version of the panel clustering method for a sparse representation of boundary integral equations. Instead of applying the algorithm separately for each matrix line (as in the classical version of the algorithm) we employ more general block partitionings. Furthermore, a variable order of approximation is used depending on the size of clusters. We apply this algorithm to a second kind Fredholm integral equations and show that the complexity of the method only depends linearly on the number, say N , of unknowns. The complexity of the classical matrix oriented approach is $O(N^2)$ while, for the classical panel clustering algorithm, it is $O(N(\log N)^7)$.

WAVELET APPROXIMATION OF BOUNDARY INTEGRAL OPERATORS

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Boundary integral formulations offer an appropriate tool for the numerical solution of certain boundary value problems in engineering. A major drawback of this approach is the fact that the arising system matrices are densely populated., Like panel-clustering and multi-pole expansion, biorthogonal wavelet bases remedy this situation by approximating the discrete scheme in an efficient way. Multi-scale methods achieve this by approximating the system matrix relative to a biorthogonal wavelet basis by a sparse matrix. We propose a fully discretized Galerkin Wavelet Method to discretize boundary integral equations which is based on parametric surface representation. The surfaces are assumed to be piecewise analytic and parametrized over quadrilateral surface (macro-)elements. Trial functions are supposed to be globally continuous and piecewise bilinear or constant in each parameter domain. We apply a first construction due to Dahmen and Schneider of biorthogonal wavelet basis on domains and manifolds with desired vanishing moments on each surface (macro-)element. Additionally, preconditioning is rather simple due to the additive Schwarz decomposition of functions with respect to different scales. We compute a sparse approximation of the system matrix directly causing only an error proportional the optimal error bound of the Galerkin discretization. This can be done such that the total number of nonzero matrix coefficients increases only linearly with the total number of unknowns N . In order to compute the nonzero matrix coefficients directly, we apply an adaptive quadrature method, with the desired accuracy requiring totally $\mathcal{O}(N)$ floating point operations. Finally we consider an application of this method to the FEM/BEM coupling.

POSTPROCESSING OF NONCONFORMING FE SOLUTIONS AND A POSTERIORI ERROR ESTIMATION

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For mathematical reasons, it is sometimes useful to weaken the continuity requirement of finite element approximations and to work with nonconforming finite elements. An example is the Stokes or Navier-Stokes problem where standard low-order conforming element pairs do not satisfy the Babuška-Brezzi stability condition. Here the nonconforming P_1/P_0 element pair of Crouzeix and Raviart satisfies that condition and provides an optimal order of convergence. Moreover, an advantage of this nonconforming element pair is that each degree of freedom belongs to at most two elements which simplifies the local communication for a parallelization of the method particularly in the 3D case.

However, for practical reasons (e.g. graphical postprocessing), one wants to have a finite element approximation of the solution which is “nice” in some sense, i.e. which is at least continuous. The obvious idea used in practice is to compute in a postprocessing step from a solution u_h^N in a given nonconforming FE space V_h^N an approximation u_h^C in some desired conforming FE space V_h^C . In this talk, we define a general transfer operator $R_h : V_h^N \rightarrow V_h^C$ for an arbitrary pair of spaces V_h^N and V_h^C . This operator is based on averaging of local nodal functionals and the computation of $u_h^C = R_h u_h^N$ can be implemented efficiently. We prove local and global estimates for the error between the exact solution u and the conforming approximation $R_h u_h^N$ in the L^2 -norm and the H^1 -seminorm.

The computable quantities η_K^{post} , being defined as the local norms of the “postprocessing error” $u_h^N - R_h u_h^N$ on the elements K , can be used for a posteriori error control. For a model problem, we derive an a posteriori error estimator for the error $u - R_h u_h^N$ which contains the quantities η_K^{post} . Results of numerical experiments are presented.

SUPERELEMENTS FOR ACCURATE SOLUTIONS TO 2-D ELLIPTIC PROBLEMS WITH SINGULARITIES ON THE DOMAIN BOUNDARY

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A novel singular superelement (SSE) formulation has been developed to overcome the loss of accuracy encountered when applying the standard finite element schemes to 2-D elliptic problems possessing a singularity arising from a re-entrant corner on the boundary or an abrupt change in the boundary conditions. The SSE consists of an inner region over which the asymptotic series of known form for the solution in the vicinity of the singular point is utilised, and a transition region over which blending functions are used to provide a smooth transition to the usual linear or quadratic isoparametric elements used over the remainder of the domain. Solution of the finite element equations also yields the coefficients in the asymptotic series directly. Numerical examples using the SSE for the Laplace equation and for computing stress-intensity factors (which are just the coefficients in the asymptotic series) in the linear theory of elasticity are given, demonstrating that accurate results can be obtained for a moderate amount of computational effort [1].

A modified version of the SSE was also designed to determine the eigenvalues of the Laplacian over domains containing re-entrant corners, and was applied to determine cut-off frequencies for TE and TM modes in electromagnetic waveguides [2]. The results compared favourably with those previously obtained by other methods of less general application. The accuracy of the results was also checked by comparing with the eigenvalues obtained using the p-version of the FEM with geometric refinement near the singularity. The p-scheme required roughly double the number of degrees of freedom

used by the current method for a given accuracy of the eigenvalues. The method was also applied to determine the lowest frequencies of acoustic vibrations in a simple 2-D model of an automobile interior.

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ADVANCED BOUNDARY ELEMENT ALGORITHMS

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We review recent progress in so-called “fast” boundary element algorithms for problems in R^3 . We present basic concepts behind wavelet-based BEM as well as so-called clustering BEM (which unify panel clustering and Fast Multipole Accelerations). Both classes of algorithms have a proved asymptotic complexity of $O(N(\log N)^a)$ with some small $a \geq 0$ where N denotes the number of degrees of freedom on the boundary. Implementations of these algorithms which exhibit this $O(N(\log N)^a)$ complexity already for moderate N are discussed. Both clustering and wavelet algorithms allow BEM-calculations with $N = 10^5 - 10^6$ DOF on workstations. Performance results are presented. A first comparison of the relative merits of wavelet-BEM and the Clustering-BEM also with standard BEM is made. Open problems and future developments are discussed.

The present work was performed jointly with Ch. Lage and is supported under the TMR network “Wavelets and Multiscale Methods in Numerical Analysis” by the EC as well as by ABB Corporate Research Center, Germany.

HIERARCHICAL HOMOGENIZATION OF COMPOSITES BY THE GENERALIZED P-VERSION OF THE FEM

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The efficient numerical modelling of laminated composites has received increasing attention in recent years – examples are sandwich plates and shells, fiber-reinforced composites and the like.

While global response to external loadings can be reliably assessed on the basis of averaged, or homogenized, models, interlamina stresses can only be obtained by resolution of the small scales of the problem.

This requirement of SCALE RESOLUTION and the low solution regularity at the matrix-composite interface seems to conflict with the use of high order, spectral or hp-FE approaches which is commonly based on large elements with smooth shape functions of high order.

We present a new approach which is able to exploit the microstructure of the material and realizes exponential convergence independently of the number of layers in the sandwich/ the number of fibers per unit length. It is based on a new spectral approach to homogenization and on nonpolynomial shape (or director) functions in the Finite Element Analysis.

For problems of the type $-\operatorname{div}(A(x/\epsilon)\operatorname{grad}u) = f$ with analytic f exponential convergence can be proved independent of ϵ .

Numerical results for a composite material and for sandwich shells will be discussed.

SIMULATIONS OF BATCH SEDIMENTATION ON THE PARTICLE LEVEL

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We present a coupled finite-difference-tracer scheme capable of resolving to satisfactory accuracy the flow around particles immersed in incompressible (Newtonian) fluids at particle Reynolds numbers of up to ≈ 15 and volume fractions below about 0.3 In dynamic simulations (2D and 3D) we measure phenomenological relations for the mean settling velocity in mono- and bidisperse suspensions and compare to experimental results and theoretical predictions for the Stokes regime ($Re \rightarrow 0$).

A POSTERIORI ERROR ESTIMATES IN THE ADAPTIVE FINITE ELEMENT METHOD OF LINES FOR PARABOLIC EQUATIONS

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A posteriori error estimates form a reliable basis for adaptive approximation techniques for modeling various physical phenomena. The estimates developed recently in the finite element method of lines for solving a parabolic differential equation are simple, accurate, and cheap enough to be easily computed along with the approximate solution and applied to provide the optimum number and optimum distribution of space grid nodes.

The contribution is concerned with a posteriori error estimates needed for the adaptive construction of a space grid in solving an initial-boundary value problem for a nonlinear parabolic partial differential equation by the method of lines. It generalizes, in some respect, previous results concerned with the semidiscrete case.

Numerical examples are presented.

MODELLING AND FINITE ELEMENT ANALYSIS OF APPLIED VISCOELASTICITY PROBLEMS

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Polymeric materials play an important role in the deformation behaviour of composite structures, particularly in modifying their damping characteristics. The task of producing realistic mathematical models of such behaviour, together with effective numerical techniques for their numerical simulation, presents a stern challenge.

In the lecture the quasistatic problem will be modelled in terms of an elliptic Volterra equation involving a history integral. A review will then be given of constitutive relations and internal variable methods that are involved in reaching this model. Numerical schemes for discretising the model will then be described, which involve space-time finite element methods. These enable *a priori* and *a posteriori* error estimates to be derived, and adaptive finite element solvers to be developed. Examples of spatially adaptive solutions will be given.

The extension of all these models and techniques to the dynamic case will then be discussed.

**DOMAIN DECOMPOSITION ITERATIVE METHODS
FOR TIME-HARMONIC MAXWELL'S EQUATIONS BASED
ON NONCONFORMING MIXED FINITE ELEMENTS**

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We present a nonconforming mixed finite element method for the approximate solution of the time-harmonic Maxwell equations in a three-dimensional, bounded domain with absorbing boundary conditions on artificial boundaries. We propose domain-decomposition iterative algorithms which are naturally parallelizable and are based on hybridizations of the mixed method. Convergence results for the iterative procedures are proved by introducing pseudo energies. The spectral radii of the iterative procedures are estimated. Numerical results are presented to compare convergence rates.

**LOW ENERGY BASIS PRECONDITIONING FOR
UNSTRUCTURED SPECTRAL/HP ELEMENT METHODS**

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We consider an *hp* discretisation of the Navier-Stokes equations in three dimensions, as applied in the unstructured solver Nektar. After apply a time discretisation which decouples the viscous and inviscid parts of the operator, the most computationally intensive part of the solver are a series of three elliptic solves, one Poisson solve and three Helmholtz solves, which are performed at each time step. Each of these elliptic solves is preconditioned with an iterative substructuring type domain decomposition method, which takes advantage of the natural splitting of the basis into interior, face, edge, and vertex basis functions.

As noted by several authors, special care must be taken in three-dimensions in order to produce a method which is scalable with respect to *h* and *p*. In particular, we propose a set of numerically evaluated low-energy basis functions calculated by solving a local elliptic problem on a regular reference element which is then mapped onto the global elements that constitute the solution mesh. The resulting method is quasi-optimal in terms of iteration count but is computationally efficient due to its local construction.

In addition we will demonstrate the efficiency of the method in a set of numerical experiments. In particular we will show that for the solution of a standard Poisson equation the low-energy preconditioner significantly reduced the number of iteration

counts as well as producing a factor of three improvement in the computational solve time.

AN EFFICIENT IMPLEMENTATION OF THE DTN BOUNDARY CONDITION FOR ACOUSTIC SCATTERING

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One method of handling acoustic problems posed in exterior (infinite) domains is to compute only on a truncated domain with a boundary condition imposed on the truncation surface. For the solution on the truncated domain to coincide exactly with the solution of the original problem, the boundary condition to be imposed is the so-called Dirichlet-to-Neumann (DtN) map. This mapping is nonlocal, meaning that the Neumann data of the solution at any point is a function of its Dirichlet data everywhere on the truncation surface. From a computational point of view, the non-locality of the DtN map is problematic because it leads to the fill in of dense blocks in the coefficient matrix of the linear system computed from a finite element modeling of the problem. These dense blocks can greatly increase the cost of computing the solution.

Several schemes have been proposed for approximating the DtN map with a local boundary condition, thus preserving the usual sparsity of the coefficient matrix in the finite element method. Unfortunately, these approximations often fail to provide sufficient accuracy. Here I will discuss an implementation of the DtN boundary condition that involves the use of a simple, local approximate boundary condition, and so preserves the sparsity of the coefficient matrix. However, in this scheme one has to solve the problem for additional right-hand sides, the final solution being a linear combination of those right-hand sides. The main advantage is that it is computationally more efficient to solve a sparse system for additional right-hand sides than it is to solve a system with dense blocks for a single right-hand side. Some examples are presented to demonstrate the accuracy and efficiency of the proposed method.

ON THE COUPLING OF FINITE AND BOUNDARY ELEMENTS

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In this talk we consider two different approaches for the coupling of finite and boundary element methods, i.e., the coupling via domain decomposition as well as via a fictitious domain method. Besides a detailed description of both formulations we will focus on the topic of preconditioning of the resulting linear systems, i.e., for degenerating subdomains and in case of local mesh refinement.

COMPUTING FLUID-STRUCTURE INTERACTION WITH TWO-DIMENSIONAL TREFFTZ-TYPE FINITE ELEMENTS

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Trefftz-type elements, or T-elements, are nonconforming finite elements the internal field of which fulfills the governing differential equations of the problem *a priori* whereas the prescribed boundary conditions and the interelement continuity must be enforced by some suitable method. Here, the relevant matching is achieved by means of a least-squares procedure. The required accuracy of the solution can be obtained by increasing the number of either the subdomains or T-functions, which can be regarded as the *h*- or *p*- type approach, respectively. The most attractive features of the formulation are its simplicity and robustness. The matrix of the resulting linear system is always Hermitian and positive definite (also for problems whose associated quadratic form is not).

Aspects related to scattering of waves by offshore structures governed by Helmholtz's equation in an unbounded 2-D domain are addressed. Different T-elements comprising those making use of suitable special purpose functions (for a doubly connected domain with a circular hole and for an angular corner subdomain) are introduced and investigated. The Sommerfeld radiation condition is also readily incorporated in the trial functions. Convergence studies are performed with much attention to the use of special purpose elements.

Some practical results for wave induced loads on the offshore, seabed, cylindrical structures are given. Our approach has led to sufficiently accurate solutions for only few subdomain division due to the fact that the oscillatory nature of wave is inherent in all kinds of Bessel functions, and as a consequence in contrast to a polynomial approximation, the dimension of the T-subdomain need not be related in any way to the wavelength. The computational results for an array of four square vertical cylinders illustrate the effects of "wave trapping" in the interior of the array.

THE INTRINSIC NORM FINITE ELEMENT METHOD FOR CONVECTION-DIFFUSION PROBLEMS

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We give a new variational analysis for convection-diffusion problems that enables one to work within the classical framework used for standard elliptic problems. This leads to a new finite element method that is quasioptimal (in the classical sense), uniformly in the diffusion parameter, with respect to a certain intrinsic norm defined by Sobolev space interpolation. We discuss the implementation of this method and show that in the case of a continuous piecewise linear trial space it is essentially the same as the streamline diffusion finite element method. This observation enables us to prescribe an optimal value (with respect to our intrinsic norm) for the free parameter in the streamline diffusion method when piecewise linears are used; up to now no optimal value for this parameter (with respect to any norm) was known.

HP-FINITE ELEMENT METHODS FOR HYPERBOLIC PROBLEMS

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We consider the error analysis of stabilised hp -finite element approximations to partial differential equations with non-negative characteristic form.

In the strictly hyperbolic case, optimal order error bounds are derived for the hp versions of the streamline diffusion finite element method and the discontinuous Galerkin finite element method.

By concentrating on the discontinuous Galerkin finite element method, we then discuss extensions of these results to second-order partial differential equations, including convection-dominated diffusion problems, degenerate elliptic equations, and second-order problems of mixed elliptic-hyperbolic-parabolic type.

The theoretical findings are illustrated by numerical experiments.

This lecture is based on joint research with Christoph Schwab (ETH Zürich) and Paul Houston (University of Oxford).

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DAMAGE MECHANICS AND PLASTICITY APPROACHES FOR TUNNELS IN JOINTED ROCK

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Rock masses are seldom found in nature without joints or discontinuities. It is the presence of these joints that makes the mechanical behaviour of jointed rock mass significantly complicated. Anisotropy, dilatancy, irreversible strain and strongly path-dependent stress-strain relations, which is generally associated with the existence of a great deal of micro- and meso-cracks and their propagation, are examples of the complex behaviour of jointed rock mass. The numerical analyses supporting tunnelling design in rock mass will in future have a better reliability only if the constitutive modelling of jointed rock is considerably improved.

In this paper, the classical plasticity approach and the recent damage mechanics approach are presented to describe the behaviour of jointed rock mass. A failure and yield criteria is an important item needed to establish an elasto-plastic model for the jointed rock. Hoek and Brown's (HB) criterion is considered appropriate for a jointed rock mass as it involves the rock quality data as reflected by the constants m and s . The criterion has been discussed comprehensively along with the characteristics of its parameters. Numerical example is given to check the results of HB criterion with the well known Mohr-Coulomb (MC) criterion. On the other hand, continuum damage mechanics, which employs some continuum variables to describe the micro-defects, has been an appealing framework for modelling geomaterials. In this study, we are attempting to put all salient features of rock mass only into the starting points: the damage variable, equivalent state and free energy function. Moreover, the geological data regarding the orientation and intensity of joint sets is used along with the suggested damage model which increase the practical importance of the damage model. Finally, a full scale tunnelling problem, San Rafael (Bolivia), is analyzed using both plasticity and damage mechanics approaches. The comparison of results of both approaches reflects the limitations of HB usage and the points of favour of the damage model.

STREAMLINE-DIFFUSION METHOD FOR NONCONFORMING AND CONFORMING ELEMENTS OF LOWEST ORDER

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We compare the convergence properties of low order finite element approximations of the streamline-diffusion method [3] applied to convection-diffusion problems. Our discussion covers both conforming and nonconforming finite elements on triangular and quadrilateral meshes. In the nonconforming case special jump terms have to be added to guarantee the stability and the same $O(h^{3/2})$ error estimate for smooth solutions [1, 2]. However, these jump terms can be avoided in the case of the nonconforming Q_1^{rot} elements on rectangular meshes [4]. Numerical experiments confirm the theoretical results and show that the technique in [5] for proving the $O(h^2)$ convergence in the L^2 -norm, cannot be applied to nonconforming elements.

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THE ADER APPROACH FOR CONSTRUCTING ADVECTION SCHEMES OF ARBITRARY ACCURACY

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A new approach (ADER) for constructing finite volume advection schemes in one, two and three space dimensions is presented. The results available so far apply to linear hyperbolic systems with constant coefficients and this paper is restricted to the scalar case in one and two space dimensions. The schemes are explicit, one-step, fully discrete and of arbitrary accuracy. The essence of the approach is to use high-order reconstructions of the data and then define a sequence of Riemann problems for all the derivatives of the reconstructed data. By applying the relevant result that *all spacial gradients obey the original evolution equation* we pose and solve derivative-Riemann problems to provide all the terms of the intercell numerical fluxes. Examples to be presented include schemes of 10th order of accuracy. Comparison with ENO and other schemes are presented. Possible ways of extending the schemes to non-linear hyperbolic systems such as the Euler equations are also discussed.

A NEW MOVING MESH ALGORITHM FOR FINITE ELEMENT CALCULATIONS I: VARIATIONAL PROBLEMS

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The idea of seeking a mesh that minimises a discrete energy functional has a relatively long history in the finite element literature. The perceived drawbacks of this approach are, firstly, the computational complexity of solving the resulting nonlinear optimisation problem and, secondly, the lack of robustness which manifests itself in mesh tangling. We shall describe a new mesh movement methodology that successfully overcomes these difficulties. In essence, our approach consists of solving a succession of local problems in such a way that, as the mesh and the corresponding discrete solution are updated, the energy functional is reduced monotonically. Applications to linear and nonlinear variational problems will be discussed.

FINITE ELEMENT MATRICES AND A *PRIORI* ERROR ESTIMATES

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The paper establishes a close relationship between Finite Element (FE) interpolation errors and properties of certain FE matrices. The proposed *a priori* error estimates are formulated in terms of eigenvalues or singular values of element stiffness matrices or "edge shape matrices". Although these estimates are algebraic in nature, they have clear geometric implications.

First, we show that the element-wise interpolation error in a given energy norm can be estimated via the maximum eigenvalue (or trace) of the stiffness matrix. This estimate is valid under fairly general and reasonable assumptions and is applicable to first or higher order triangular or tetrahedral elements, as well as to elements of other types.

In many cases, the maximum eigenvalue has a clear geometric meaning. In particular, Zlámal's minimum angle condition and the Syng-Babuška-Aziz maximum angle condition for first order triangular elements follow from the maximum eigenvalue criterion. Even without a geometric interpretation, the eigenvalue / trace condition is useful in practical FE computation, as the matrix traces are available at virtually no additional cost. Moreover, the stiffness matrix automatically reflects the chosen energy norm, possibly for anisotropic parameters.

Applied to interpolation of conservative fields on Nedelec's edge elements, the maximum eigenvalue analysis ultimately leads to a new criterion. For the energy-seminorm approximation on first order tetrahedral nodal elements, or equivalently, for L_2 -approximation of conservative fields on tetrahedral edge elements, the interpolation error is proved to depend on the minimum singular value of the 'edge shape matrix' whose columns represent the unit edge vectors of the tetrahedron.

The new singular value estimate is a precise and clear generalization of the maximum angle condition to three (and more) dimensions. Multiple links between the minimum singular value and the standard geometric measures (angles, the ratio of the radius of the inscribed sphere to the element diameter, etc.) are established. The minimum singular value condition is proven to be not only sufficient, but in some strong sense necessary for the convergence of FE interpolation on a family of meshes.

The results are illustrated with numerical experiments.

A FINITE VOLUME METHOD FOR VISCOUS COMPRESSIBLE FLOWS FOR LOW AND HIGH SPEED APPLICATIONS

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Discretization methods for viscous compressible flows lead to systems of equations which become stiff in two typical flow situations. First, near walls, in high Reynolds number applications, high aspect ratio cells are necessary to capture the boundary layer. This leads to numerically anisotropic behaviour of the acoustic and the diffusive terms. Second, in low speed regions of the flow, the ratio of the convective and acoustic eigenvalues of the inviscid system becomes very high.

We implemented an AUSM (Advection Upstream Splitting Method) based discretization method, using an explicit third-order discretization for the convective part, a line-implicit central discretization for the acoustic part and for the diffusive part. The lines are chosen in the direction of the gridpoints with shortest connection. The semi-implicit line method is used in multistage form because of the explicit third-order discretization of the convective part. Multigrid is used as acceleration technique. Due to the implicit treatment of the acoustic and the diffusive terms, the stiffness caused by high aspect ratio cells is removed.

The low Mach number stiffness is treated by a preconditioning technique. To ensure physical correct behaviour of the discretization for vanishing Mach number, extreme care has to be taken. For vanishing Mach number, stabilization terms have to be added to the continuity and the energy equation. In the energy equation, pressure stabilization is necessary, leading to a Laplacian-like term in pressure. In the continuity equation pressure and temperature stabilization terms are necessary. The coefficients of these terms have been constructed so that correct scaling with Mach number is obtained.

The purpose of the paper is to present a scheme which reaches high quality and high efficiency independent of Mach number. Several examples of flows are discussed. It is demonstrated that the convergence is very good, independent of grid aspect ratio and Mach number.

AN INVESTIGATION OF MESH QUALITY AND ANISOTROPIC MESH REFINEMENT FOR SOME FINITE ELEMENT METHODS FOR FLUID FLOW

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It is common for the choice of a suitable mesh for a problem to be handled automatically by modern finite element software. Error estimates typically measure the accuracy of the solution represented on the mesh and indicate where refinement may improve the solution quality. A related but less often considered issue is whether the error estimate can directly reflect the suitability of the mesh for the problem as well as the accuracy of the solution itself.

Examination of a finite element method for the extended Boussinesq shallow water wave equations illustrates that the quality of the numerical solution can be strongly dependent on the choice of an appropriate mesh for the problem.

A second example considered is the three-dimensional scalar advection equation. To account for the presence of discontinuous and near-discontinuous features a Galerkin Least-Squares finite element method is used. Reliable error estimates have been developed for finite element methods for this equation and sufficient isotropic refinement of the mesh, typically uniform subdivision of the elements, will produce accurate solutions. However in three dimensions this can lead to an excessively large mesh. Typical solutions of this equation have layers that vary rapidly in only one direction, naturally suggesting a similar directional refinement of the mesh. Some of the error estimation procedures that have been used for these problems are illustrated for a model solution of the advection equation.

Use of anisotropically adapted meshes necessitates the development of reliable error estimates that include directional information. Developments in this area are reported on and an outline of the work proposed for this project is presented.

A FINITE ELEMENT BASED APPROACH FOR NONLINEAR, UNSTEADY FLUID STRUCTURE INTERACTION PROBLEMS

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This study is focussed on the time-dependent solution of coupled motions of geometrically nonlinear structures and viscous incompressible Newtonian fluids. Typical areas of application, which could be appropriately described with these models, are liquid-filled storage tanks under strong excitations like earthquake motion, wind-induced vibrations of chimneys, bridge girders or cables etc.

The present computational approach is completely based on finite elements for the spatial discretization. The space time relation is adopted in a semi-discretization approach employing different direct time integration schemes.

The cases under study involve large structural displacements at small strains and therefore geometrically nonlinear effects have to be taken into account for the structural part. These large structural displacements also seriously effect the description of the fluid domain. For an appropriate handling of such moving boundary problems (deforming interfaces, free surfaces) the basic conservation equations for the fluid, namely the instationary, incompressible Navier-Stokes equations, are reformulated within an Arbitrary Lagrangean-Eulerian (ALE) framework. In order to tackle arising numerical problems when using standard finite element strategies to this kind of flow problems a special fully stabilized ALE finite element method has been developed.

Assembling the above components of this physical two-field system leads to a computational three-field coupled problem. The third field, a purely computational field, is introduced by the moving mesh and stems from the reference domain, introduced through the ALE kinematic description. The three-field coupled problem is solved via a partitioned analysis approach especially focussing on loose, i.e. sequential staggered, coupling schemes. Recently developed, improved staggered time-integration schemes can be shown to give stable and more accurate results at roughly the same computational costs as standard staggered integration procedures. In addition questions of the interrelation of the applied single-field time-integrators and the significance of so-called Geometric Conservation Laws are addressed.

First selected numerical examples demonstrate the performance of the overall computational procedure. The range of examples includes channel flows with flexible walls, that can be used as simplified models to study blood flow in arteries, as well as large, vortex-induced oscillations of highly flexible structures.

CONTACT ELEMENTS IN THE STRESS ANALYSIS OF INTRAMEDULLARY NAILS

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Over the last few decades there have been major advances in the surgical use of biomechanical implants, and such developments have made major impacts on the quality of life of many patients. One of these developments has been the use of intramedullary nailing in the treatment of unstable hip fractures and in particular of inter-, per- and sub-trochanteric fractures. These surgical developments have not always been associated with appropriate predictive analysis resulting in short-comings in the performance of the devices. However, Osteo AG have sponsored work on the development of finite element modelling to predict the behaviour of intramedullary nails in new applications, and to investigate the optimisation of design parameters and surgical practice in certain predictable conditions. Intramedullary nailing involves the use of a nail fitted into the medullary canal of a long bone. This proximal femur nail is usually held in the bone by one or two distal locking screws. The femur head may be secured to the nail by using one or two lag screws. The nail is available in different sizes, and contact occurs between the nail and the inside of the femur, and between the nail and the screws securing it. The key variables include the material properties (bone is a highly variable non-isotropic material, while there are several alternatives for the nail), the geometry of the nail, and the loading on the femur, as well as the contacts generated. There are several proprietary makes of nail, but this study seeks to investigate key parameters such as flexural rigidity of the distal end of the nail, and the layout of the screws. The distal (lower) end of the nail is tapered to make the surgical procedure viable and the load sharing of the distal end of the nail and the distal screw(s) will depend on the contacts generated. Contacts as a result of small deformations may also determine the load sharing characteristics if more than one screw is used. The contacts generate local high stresses in the region of the screws, and where failures have occurred in practice, they have been found mainly in the vicinity of the screws, in the nail, screw or bone. The results presented here show the modelling (using commercially available F.E. code) and analysis of this problem, along with some key results from implementation. In particular, details of the mechanisms selected to model the contact are presented. The presentation will draw some general conclusions about F.E. modelling in this context, and outline some of the developments necessary to improve the modelling and validate the results.

HYBRID, NEURAL-NETWORK/FINITE-ELEMENT ANALYSIS OF ELASTOPLASTIC PLATES

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The neural network (NN) can be used as a quick simulator to map input to output data without knowing ‘*a priori*’ the relation between them. The main problem of NN preparing for operation is training network on known examples. The NN trained off-line can be used as an efficient neural procedure instead of a complex numerical procedure. This can be of value for procedures associated with the analysis of constitutive equations.

The paper develops the idea concerning implementation of hybrid NN/FE programs for the analysis of elastoplastic problems. Two such problems are discussed: A) plane stress problem, B) plate bending problem. In both problems a simple model of material is assumed, corresponding to isotropic and homogeneous material with J_2 yield surface and isotropic strain-hardening. The constitutive equations obey the classical flow theory. Linear kinematic and equilibrium equations are assumed.

The back-propagation neural network (BPNN) is used for formulating neural procedures. The first procedure is implemented for the simulation of the return mapping algorithm, the second procedure for the elastoplastic bending analysis at cross-sectional level.

Patterns for the BPNN procedures were computed by ANKA FE code [1]. In case of plane stress only constitutive relations were used. Patterns for the bending analysis had to be based not only on constitutive equations but also Kirchhoff’s kinematic hypothesis was taken into account. Due to constitutive-supported patterns the implemented neural procedures can be used for various boundary conditions, plate shapes and loads applied.

Problem A) is illustrated by two examples. The first one deals with a perforated plate, the second one analyses a notched beam. The computations show that the hybrid program ANKA-H2 can analyse different special cases using 50-70% of processor time needed for the execution of purely FE code ANKA.

Problem B) was used for the analysis of rectangular plates with different material strain-hardenings, different boundary conditions and load distributions.

It can be concluded that due to “objective” patterns used for the neural procedures training the corresponding hybrid BPNN/FEM programs are much more general than the hybrid programs related to “subjective” procedures [2, 3]. On the other hand the subjective procedures (related to a special case of plane stress or to a selected bending plate) enable us to formulate simpler neural procedures. This can influence the efficiency of hybrid programs, especially related to the plate bending.

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LOCALLY CONSERVATIVE ALGORITHMS FOR FLOW

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In the numerical modeling of fluid flow and transport problems, it is necessary for the velocities to be locally conservative on the transport grid. Lack of local mass conservation results in spurious sources and sinks to the transport equation. Local mass conservation can be accomplished through a projection algorithm, but this can be expensive and is generally only first order. It is generally better to use a locally conservative approach from the beginning.

Here we describe several numerical locally conservative algorithms: discontinuous Galerkin methods, mixed finite element methods, and control volume. We discuss advantages and disadvantages of each of these methods. Numerical results from subsurface and surface flow problems are presented.

A MORTAR FINITE ELEMENT METHOD USING DUAL SPACES FOR THE LAGRANGE MULTIPLIER

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The mortar finite element method allows the coupling of different discretization schemes and triangulations across subregion boundaries. In the original mortar approach the matching at the interface is realized by enforcing an orthogonality relation between the jump and a modified trace space which serves as a space of Lagrange multipliers. Here, the Lagrange multiplier space is replaced by a dual space without losing the optimality of the method. The advantage of this new approach is that the matching condition is much easier to realize. In particular, all the basis functions of the new method are supported in a few elements. The mortar map can be represented by a diagonal matrix; in the standard mortar method a linear system of equations must be solved. The problem is considered in a positive definite nonconforming variational as well as an equivalent saddle-point formulation. The efficient iterative solver of the discrete problem is based on a multigrid method for a nonsymmetric problem on the unconstrained product space.

ON *H*-ADAPTIVE FINITE ELEMENT METHODS CONTACT PROBLEMS

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Adaptive finite element methods have been developed over the last ten years for engineering problems in solid and fluid mechanics. They provide a tool for accurate and reliable analysis which is needed in many application. The use of these techniques within contact problems is advantageous since the contact area is not known a priori and thus element sizes cannot be estimated beforehand.

Within this contribution we develop different adaptive finite element techniques for continuum and shell problems undergoing finite deformations including elasto-plasticity. Two or more deformable bodies are allowed to come into contact. During the analysis the contact is assumed to be frictionless.

Different adaptive methods are considered which base on the development of new error indicators and error estimators related to the contact area. Based on these quantities numerical methods are constructed which allow automatic mesh refinement for two and threedimensional continuum and shell problems. Several examples are discussed which depict different convergence behaviour of the developed schemes.

INTEGRAL EQUATION FORMULATIONS FOR THE LOW REYNOLDS NUMBER DEFORMATION OF VISCOUS FLUIDS UNDER SURFACE TENSION

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This paper presents novel integral equation formulations to study the deformation of a slow viscous flow in a bounded fluid region under surface tension, and containing features such as air bubbles, drops of fluids of different viscosity, or rigid inclusions. The formulations are based on boundary integral equations of the second kind in terms of only one surface potential. It is shown that, in order to provide unique solutions, these integral representations should be completed by the addition of terms that give arbitrary total force and torque in suitable linear combinations.

The formulations have application to problems of viscous sintering, a process for manufacturing of high quality glass by means of sol-gel processing. Sintering is a process in which a granular compact of metals, ionic crystals or glasses consisting of many particles, is heated to such a temperature that the mobility of the material becomes sufficient to make contiguous particles coalesce. In the production of aerogels and glassy materials, the material transport can be modelled as a viscous incompressible

Newtonian flow, driven solely by surface tension.

The theoretical background to the technique is explained in detail, including mathematical proofs of existence and uniqueness of solutions. Numerical results of simple test problems are included to validate the formulations.

LAGRANGIAN FINITE VOLUME ANALYSIS OF GLASS PRESSING

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A fully Lagrangian Finite Volume method on unstructured triangular meshes for the analysis of glass pressing is developed. Lagrangian form of Navier -Stokes equations are used to model the axi-symmetric, incompressible, Newtonian flow of glass during pressing. The well known SIMPLER algorithm is used for the pressure-velocity coupling. The mesh is smoothed at each time step and is regenerated automatically when distorted too much. Accuracy of the method is assessed by comparison of solutions of simple test problems. The method is applied to simulation of practical glass pressing process.

EXTRACTING CERTAIN QUANTITIES ASSOCIATED WITH THREE-DIMENSIONAL SINGULARITIES IN ELLIPTIC BVP BY P-FEM

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A numerical method is described for the computation of eigen-pairs and edge flux/stress intensity functions which characterize the exact solution of elliptic boundary value problems (Laplace and Elasticity equations will be addressed) in three-dimensions in the vicinity of edges. These may be caused by re-entrant faces or abrupt changes in material properties.

Such singularities are of great interest from the point of view of failure initiation: The eigen-pairs characterize the straining modes and the edge flux/stress intensity functions (EFIFs/ ESIFs) quantify the amount of energy residing in particular straining modes. For this reason, failure theories directly or indirectly involve the eigenpairs and EFIFs/ESIFs.

The problem of determining the eigen-pairs numerically on the basis of the modified Steklov formulation (presented in [1]) in conjunction with the p-version of the finite element method is presented. The weak eigen-problem for determining eigen-pairs is formulated both for edge and vertex singularities.

For edge singularities, the edge is excluded from the domain over which the integral is computed, and a *two-dimensional* sub-domain is constructed in a plane perpendicular to the edge. Thus high-order finite element methods provide exponential convergence rates for the eigen-pairs. Numerical results are provided for several cases in elasticity

including isotropic as well as anisotropic multi-material interfaces.

Several methods for extracting the EFIFs/ESIFs from the finite element solution will also be addressed. Methods as the L^2 and energy projection methods will be analyzed, and an adaptive scheme based on the dual weak form will be described if time allows.

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BOUNDARY LAYERS IN THIN ELASTIC 3-D DOMAINS VIS 2-D HIERARCHIC PLATE MODELS

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Plates are viewed in structural engineering practice as three-dimensional components with one of their dimensions, usually denoted by "thickness", much smaller compared to the other two dimensions. Due to the complexity of a three-dimensional elastic analysis, much attention has been given historically to the derivation of "plate-models", which can be understood as an application of dimensional reduction principles. These are aimed to approximately solve the three-dimensional problem by a two-dimensional formulation.

The quality of a plate-model must be judged on the basis of how well its exact solution approximates the corresponding three-dimensional problem. Especially, of much interest are the boundary layers which may occur in a three-dimensional plate, and their realization (if possible at all) in plate-models.

This talk addresses the behavior of the linear elastic solution in three-dimensional thin domains near the boundaries, and compare it to the approximated solution obtained by dimension reduced 2-D hierachic plate models. Numerical simulations using the hp-version of the finite element method are used. We quantify the engineering quantities which are rapidly changing in a boundary layer and investigate how well (if at all) the two-dimensional plate-models solutions approximate the three-dimensional solution inside and outside of the boundary layers [1]. The advantages of the hp-FEM, which make this research possible will be addressed.

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**MATHEMATICAL ANALYSIS OF ZIENKIEWICZ-ZHU
PATCH RECOVERY TECHNIQUE**

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In 1992, O.C. Zienkiewicz and J.Z. Zhu proposed a patch recovery technique. The technique recovers the gradient quantities in an element from element patches surrounding the nodes of the element. It has been shown numerically that the recovery technique provides superconvergent recovery on regular meshes and provides recovery with much improved accuracy on general meshes. In this talk, we present a survey of the theoretical investigation on this recovery technique.

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Author Index

Adjerid S., 1
Ainsworth Mark, 1
Akin J. E., 2
Amini Siamak, 3
Ammari Habib, 95
Andrä H., 4, 5
Apel Thomas, 5, 6
Arens T., 90
Armstrong C.G., 91
Arunakirinathar K., 6
Assous Franck, 7
Astley R. J., 8

Babuška Ivo, 1, 9
Bach Michael, 10
Baines M. J., 11
Banks H.T., 12
Barbone P. E., 56
Barrett K.E., 12
Barron J. R., 13
Bartoš M., 14
Beneš V., 15
Benoit C., 16
Bermúdez Alfredo, 17, 18
Berzins M., 129
Bettess P., 78
Blaheta R., 19
Boffi D., 20, 21
Brown B.M., 22
Brown C.J., 131
Bruch, Jr. J.C., 66
Burda Pavel, 15, 23
Bürger R., 24
Buyukyenerel Gultekin, 25

Carneiro O. S., 96
Casarin Mario, 120
Cecot W., 37
Chandler-Wilde Simon N., 26
Chao T.-Y., 27
Chauvière Cédric, 28
Ciarlet Jr. Patrick, 7
Cimrman R., 113
Cividini Annamaria, 29
Cliffe K. A., 30
Cockburn Bernardo, 31
Collino F., 31
Coorevits P., 16, 32

Costabel M., 33
Coyette Jean-Pierre, 34
Crawford R.J., 91
Cundev M. D., 34, 107
Cvetkovski G. V., 34, 107

Dauge M., 33
Davies E.B., 22
Dawson Clint, 36
De Schepper H., 38
de Lacerda L. A., 78
Demkowicz Leszek, 37, 65
D'Souza Karl S., 102
de Tolla Dan, 102
Dey Saikat, 39
Dick E., 128
Dický Jozef, 40
Dostál Z., 41
Durán R., 17
Düster Alexander, 111
Dutko M., 99

Erdmann B., 42
Evje S., 24

Feistauer Miloslav, 43
Feng Y. T., 44
Fey M., 45
Fish Jacob, 46
Flaherty J.E., 1
Formaggia Luca, 47
Fujii N., 64

Gaitens M.J., 12
Gallimard L., 48
Ganesh M., 49
Gastaldi L., 20, 21
Gatica Gabriel N., 50
Gawęcki Andrzej, 51
Gerdes Klaus, 52
Giebermann K., 52, 53
Gioda Giancarlo, 29
Givoli D., 53
Gómez M. D., 54
Gomez Neto F. A. M., 41
Graham Ivan G., 30, 55
Griebel Michael, 53

Ha Taeyoung, 120

Hackbusch Wolfgang, 70
 Hackl B., 55
 Hamilton J. A., 8
 Harari I., 56
 Hassan O., 94
 Hazard Christophe, 57
 Hebeker F.-K., 58
 Heinrich B., 59
 Helmig Rainer, 60
 Henshall J. L., 67
 Herrmann Hans, 118
 Heuer Norbert, 60
 Hild P., 32
 Höfler Kai, 118
 Holzer Stefan M., 61
 Houston Paul, 62
 Hsiao G.C., 63
 Huesler E.J., 131
 Hülsemann F., 63
 Ichikawa Y., 64
 Ihlenburg Frank, 65
 Jeltsch R., 45
 Jiang B., 66
 Jiang W. G., 67
 Jimack Peter K., 22, 68, 129
 Johnson A. R., 69, 119
 Joly P., 54
 Karakashain Ohannes, 69
 Karlsen K. Hvistendahl, 24
 Kawamura K., 64
 Kellogg R. Bruce, 123
 Kestřánek Z., 14
 Kestřánek jr Z., 14
 Khoromskij Boris N., 70
 Kim Mi-Young, 71
 Kirby J.A., 71
 Klawonn Axel, 72
 Kohut R., 19
 Kornhuber R., 72
 Krause R., 72
 Krause Roland, 73
 Křížek Michal, 73
 Kroener Dietmar, 74
 Kuczma Mieczyslaw S., 75
 Kuhn M., 76, 79
 Kunert G., 77
 Kwon Ohin, 120
 Ladevèze P., 48

Laghrouche O., 78
 Lang J., 42
 Langer U., 76, 79
 Lappin J., 80
 Laszloffy A., 103
 Leary S. J., 80
 Legat V., 81
 Lerch R., 76
 Lie K.-A., 24
 Lima Tiago, 34
 Lohrengel Stephanie, 57
 Long J., 103
 Lubuma J. M.-S., 82
 Lytvyn Oleg, 83
 Mahnken R., 84
 Maischak Matthias, 85
 Malhotra M., 86
 Marburg Steffen, 87
 Matthies Hermann G., 88
 Matthies G., 125
 Maurer J., 45
 Mayo Anita, 88
 McEvoy J.P., 91
 Meddahi S., 89
 Meenaghan Michael, 102
 Meier A., 90
 Melenk J. M., 90
 Menary G.H., 91
 Merci B., 128
 Migeot Jean-Louis, 34
 Mihajlović M.D., 22
 Mijalkovic S., 91
 Millington R. C., 126
 Minár Roman, 40
 Mokhtarzadeh-Dehghan M. R., 95
 Molenkamp F., 92
 Möller P., 93
 Morgan K., 94
 Moses P., 15
 Mühlhuber W., 76
 Nakano M., 64
 Natarajan S., 95
 Nédélec Jean-Claude, 95
 Nedoma J., 14
 Nejad L. A. M., 126
 Neto E. A. de Souza, 99
 Nicaise Serge, 6, 82
 Nobile Fabio, 47
 Nóbrega J. M., 96

Novotný Jaroslav, 15, 23
 Oden J. Tinsley, 97
 Ohnimus S., 98
 Owen D. R. J., 44, 99
 Owens Robert G., 28
 Pabisek Ewa, 132
 Paquet L., 82
 Park Eun-Jae, 101
 Park Jungho, 101
 Pasciak Joseph E., 101
 Patlashenko I., 53
 Patra Abani K., 102–104
 Pavarino Luca F., 105
 Pegg N. E., 94
 Pelle J.-P., 16, 32, 48
 Peric D., 44, 99
 Peszynska Małgorzata, 106
 Petkovska L. B., 34, 107
 Phillips Tim, 108
 Pinsky P. M., 86
 Pinter G.A., 12
 Plaks A., 127
 Potter L.K., 12
 Power H., 134
 Pradlová Jana, 73
 Primo A. R. M., 134
 Procter P., 131
 Profit Anthony, 3
 Quarteroni Alfio, 47
 Quatember Bernhard, 109
 Rachowicz W., 37
 Radkevich Evgeniy, 110
 Rahman M., 26
 Ramm Ekkehard, 130
 Rank Ernst, 111
 Rannacher Rolf, 111, 112
 Reed M. B., 27
 Reitzinger S., 76
 Riemslagh K., 128
 Rodríguez Rodolfo, 17, 18
 Rohan E., 112, 113
 Ross Christopher R., 26
 Rüter M., 98
 Santos Juan, 114
 Santos S. A., 41
 Sauter Stefan, 114
 Sayas F.-J., 89
 Scheichl R., 30
 Schieweck F., 115
 Schiff Bernard, 116
 Schinnerl M., 76
 Schnack E., 63
 Schneider Reinhold, 115
 Schöberl J., 55, 76, 79
 Schwab Ch., 117, 118
 Schwarzer Stefan, 118
 Segeth K., 119
 Segré Jacques, 7
 Seiki T., 64
 Sharma C. B., 92
 Shaw Simon, 119
 Sheen Dongwoo, 120
 Sherwin Spencer, 120
 Shirron Joseph J., 121
 Sidi A., 53
 Sloss J.M., 66
 Solomin J., 17
 Stals L., 30
 Starý J., 19
 Stehlík J., 14
 Stein E., 98
 Steinbach O., 49, 121
 Steindorf Jan, 88
 Stephens D. R., 2
 Stoilkov V. N., 34, 107
 Stojek Małgorzata, 122
 Stynes Martin, 123
 Süli Endre, 123
 Suttmeier F. T., 112
 Swoboda G., 124
 Tobiska L., 125
 Toro E. F., 126
 Tourigny Y., 63
 Tourigny Yves, 126
 Tsukerman I.A., 127
 Van Keer R., 38
 Veneziani Alessandro, 47
 Vierendeels J., 128
 Wachmann Bernd, 118
 Walhorn E., 98
 Walkley M., 129
 Wall Wolfgang A., 130
 Wang C.J., 131
 Warby M. K., 4, 5, 71
 Waszczyzyn Zenon, 132

Weatherill N. P., 94
Wendland W.L., 63
Wheeler Mary Fanett, 133
Whiteman J. R., 4, 5, 71, 119
Williams A. J., 108
Wohlmuth Barbara, 133
Wriggers P., 134
Wrobel L. C., 78, 134

Yanyo L.C., 12
Yettram A.L., 131
Yigitler Kayhan, 135
Yosibash Zohar, 116, 135, 136

Zhang Zhimin, 137
Zyserman Fabio, 114